The mathematics of dilute quantum gases

2. Ground state energy of the dilute Bose gas

- Definition of scattering length and the scattering equation
- Heuristics
- Upper bound - a trial state argument
- Lower bound - Dyson Lemma + rigorous version of first order perturbation theory

We follow: Lieb, Seiringer, Solovej, Yngvason, "The mathematics of the Bose gas and its condensation", Chapter 2.

1. The scattering length and the scattering equation

Let $V \in L^2(\mathbb{R}^3)$ be a nonnegative and radial function with compact support. By $R_0 > 0$ we denote the radius of its support, that is, $V(x) = 0$ if $|x| > R_0$. We call the following equation the <u>zero energy scattering equation</u>

$$-\Delta f(x) + \frac{1}{2} V(x) f(x) = 0 \quad \text{with} \quad \lim_{|x| \to \infty} f(x) = 1. \tag{1}$$

The scattering equation has a unique solution f with the following properties:

(1) f is a weak solution of (1) in the sense that

$$\int \nabla \varphi(x) \nabla f(x) \, dx + \frac{1}{2} \int \varphi(x) V(x) f(x) \, dx = 0 \tag{2}$$

holds for all $\varphi \in \mathcal{C}_c^\infty(\mathbb{R}^3)$.

(2) f is radial, that is, there exists a function $f_0 : \mathbb{R}_+ \to \mathbb{R}$ such that $f(x) = f_0(|x|)$.

(3) For $r > R_0$ we have the explicit form

$$f_0(r) = f_0^a(r) = 1 - \frac{a}{r} \tag{3}$$

for $a \in \mathbb{R}_+$. The number a is called the <u>scattering length</u>. It is a combined measure for the range and the strength of v.

(4) For $0 < r < R_0$ we have the bound

$$f_0(r) \geq f_0^a(r). \tag{4}$$

(5) The scattering length and the solution of the scattering equation are monotone in the following sense: Let $\tilde{v}$ be such that $v(x) \geq \tilde{v}(x) \geq 0$ for all $x \in \mathbb{R}^3$ and let $\tilde{f}_0(r)$ be the solution of the scattering eq. with $\tilde{v}$. Then

$$f_0(r) \leq \tilde{f}_0(r) \quad \text{for all } r > 0 \text{ and } a \geq \tilde{a} \geq 0.$$

We will later need the following energy related to f that we compute now:

$$\mathcal{E}(f) = \int_{\mathbb{R}^3} \left\{ |\nabla f(x)|^2 + \tfrac{1}{2} v(x) |f(x)|^2 \right\} dx$$

$$= \lim_{R\to\infty} \left\{ \int_{B_R(0)} f(x) \left\{ -\Delta + \tfrac{1}{2} v(x) \right\} f(x)\, dx + \int_{\partial B_R(0)} f(x) \nabla f(x) \cdot n(x)\, dx \right\}$$

The first term equals zero because f solves the scattering equation. The second term equals for $R > R_0$

$$\lim_{R\to\infty} \int_{\partial B_R(0)} \left(1 - \frac{a}{R}\right)\left(\frac{a}{R^2}\right) d\omega_R(x) = \lim_{R\to\infty} \left(1 - \frac{a}{R}\right) 4\pi a .$$

uniform measure
on unit sphere

We therefore conclude $\boxed{\mathcal{E}(f) = 4\pi a}$. (5)

2.) Preliminary discussion and heuristics

In this Chapter we are interested in proving an asymptotic formula for the ground state energy per unit volume

$$e_0(\rho, v) = \lim_{\substack{N,L\to\infty \\ N/L^3 = \rho}} \frac{E_0(N,L,v)}{L^3} \tag{6}$$

of the dilute Bose gas. Here dilute means that the scattering length a of v is much smaller than the typical distance between the particles given by $\rho^{-1/3}$. In other words, we will investigate the asymptotic behavior of $e_0(\rho, v)$ in the limit where $a\rho^{1/3}$ tends to zero (low density or dilute limit). The ground state enery $E_0(N, L, v)$ is the lowest eigenvalue of the Hamiltonian

$$H_N = \sum_{i=1}^{N} -\Delta_i + \sum_{1\le i<j\le N} v(x_i - x_j) \tag{7}$$

when restricted to the bosonic subspace $L^2_s(\mathbb{R}^{3N})$ of $L^2(\mathbb{R}^{3N})$. The precise statement we are going to prove is the following Theorem:

<u>Theorem (Low density limit of the ground state energy of the Bose gas; Lieb, Yngvason 1998; Dyson 1957, Lieb, Seiringer, Yngvason 2000)</u>

Let $v \in L^2(\mathbb{R}^3)$ be a nonnegative and radial function with compact support and assume that H_N is defined with boundary conditions that make it self-adjoint (e.g. Neumann, Dirichlet, periodic or Robin). Then the ground state energy $e_0(\rho, v)$ is in the dilute limit given by

$$\lim_{\rho^{1/3}a\to 0} \frac{e_0(\rho, v)}{4\pi a\rho^2} = 1. \qquad (8)$$

Remark 1: The statement holds more generally for $V: \mathbb{R}^3 \to \mathbb{R}_+$ a radial and measurable function s.t.

$$\int_{B_R^c(0)} V(x)\,dx < +\infty \qquad (9)$$

for some $R>0$. In particular, V can take the value $+\infty$ on a set of positive measure, which allows one to incorporate hard core interactions. The proof we are going to present applies to this more general setting.

Remark 2: It can be shown that the lowest eigenvalue of H_N on $L^2(\mathbb{R}^{3N})$ and on $L^2_s(\mathbb{R}^{3N})$ are the same. This is a general principle following from the properties of the Laplacian, see e.g. Reed, Simon, "Methods of modern mathematical physics 4, Analysis of Operators, Chapter 12".

Heuristics:

a.) Ground state energy in case $V=0$ (the ideal gas): Let

$$H_N^0 = \sum_{i=1}^{N} -\Delta_i \tag{10}$$

with periodic boundary conditions. In this case the Laplacian can be explicitly diagonalized and its complete set of eigenfunctions reads $\left\{ \frac{1}{L^{3/2}} e^{ipx} \right\}_{p \in \frac{2\pi}{L}\mathbb{Z}^3}$

with eigenvalues p^2, that is,

$$-\Delta \frac{1}{L^{3/2}} e^{ipx} = \frac{p^2}{L^{3/2}} e^{ipx}. \tag{11}$$

Exercise 1: Argue why $\left\{ \frac{1}{L^{3/2}} e^{ipx} \right\}_{p \in \frac{2\pi}{L}\mathbb{Z}^3}$ is a complete basis for $L^2([0,L]^3)$.

The eigenfunction to the lowest EV of H_N^0 is the minimizer of the following minimization problem

$$\inf_{\|\Psi\|=1} \langle \Psi, H_N^0 \Psi \rangle. \tag{12}$$

By choosing $\Psi_N^0(x_1 \dots x_N) = \prod_{i=1}^N \varphi_0(x_i)$ with $\varphi_0 = \left(\frac{1}{L}\right)^{3/2}$, we see that we can minimize each term in the sum of H_N^0 separately. We thus have $E_0(N,L,0) = 0$.

b.) <u>The concept of Bose-Einstein condensation</u>: Let $\Psi_N \in L_s^2([0,L]^{3N})$ be a sequence of bosonic wave functions and define

$$\gamma_N(x,y) = N \int_{[0,L]^{3(N-1)}} \Psi_N(x, q_1 \dots q_{N-1}) \overline{\Psi_N(y, q_1 \dots q_{N-1})} \, d(q_1 \dots q_{N-1}). \quad (13)$$

By a slight abuse of notation we denote by γ_N also the bounded operator on $L^2([0,L]^3)$ defined by

$$(\gamma_N \Psi)(x) = N \int_{[0,L]^3} \gamma_N(x,y) \Psi(y) \, dy. \quad (14)$$

Note that $\varrho_N(x) = \gamma_N(x,x) N^{-1}$ is the one-particle marginal of the N-particle probability distribution $|\Psi_N(x_1 \dots x_N)|^2$. The operator γ_N is a <u>quantum</u> marginal distribution because it allows one to compute more than just a a reduced probability distribution for the position of the particles in the gas. We e.g. have

$$\langle \Psi_N, H_N^0 \Psi_N \rangle = \int_{[0,L]^3} \left[-\Delta_x \gamma_N(x,y) \right]_{x=y} dx . \qquad (15)$$

By definition, the sequence $\{\Psi_N\}_{N=1}^{\infty}$ is said to show <u>Bose-Einstein condensation (BEC)</u> if

$$\liminf_{\substack{N,L\to\infty \\ N/L^3=\rho}} \sup_{\|\Psi\|=1} \frac{\langle \Psi, \gamma_N \Psi \rangle}{N} > 0, \qquad (16)$$

that is, if the largest eigenvalue of γ_N is of order N in the thermodynamic limit. In the case of a gas in a box one can expect that the eigenvector of the largest eigenvalue of γ_N is a constant, and hence (16) is equivalent to

$$\lim_{\substack{N,L\to\infty \\ N/L^3=\rho}} \frac{1}{L^3 N} \int_{[0,L]^6} \gamma_N(x,y)\, d(x,y) > 0 . \qquad (17)$$

Using (17) as the definition for BEC, we check that the ideal gas in the box shows BEC in the ground state. More precisely, we found that the ground state wave function of H_N^0 is given by $\Psi_0(x_1 \dots x_N) = \left(\frac{1}{L^{3/2}}\right)^N$. Its one-particle density matrix γ_N has the kernel

$$\gamma_N(x,y) = \frac{N}{L^3} = \rho. \tag{18}$$

Accordingly,
$$\frac{1}{L^3 N} \int_{[0,L]^6} \gamma_N(x,y)\, d(x,y) = 1 \tag{19}$$

and the system shows by definition complete BEC.

Remark: One expects that also the interacting ground state shows BEC. Proving this claim is a major open problem in mathematical physics for almost a century.

c.) A wrong way to estimate $e_0(\rho,\nu)$

Even if nobody can prove that there is BEC in the interacting system it might be helpful to assume BEC to prove an upper upper bound for $e_0(\rho, v)$. Because $E_0(N,L,v) = \inf_{\|\Psi\|=1} \langle \Psi, H_N \Psi_N \rangle$ we obtain an upper bound with a trial state. Let us choose Ψ_N^0 and see what we get.

$$E_0(N,L,v) \leq \langle \Psi_N^0, H_N \Psi_N^0 \rangle = \sum_{1\leq i<j\leq N} \int_{[0,L]^{3N}} v(x_i - x_j) \underbrace{|\Psi_0(x_1 \dots x_N)|^2}_{\left(\frac{1}{L^3}\right)^N} \underbrace{dX}_{dx_1 \dots dx_N}$$

$$= N(N-1) \frac{1}{L^6} \int_{[0,L]^6} v(x-y)\, d(x,y) = \frac{N(N-1)}{L^3} \int_{[0,L]^3} v(x) dx . \quad (20)$$

For the moment we have assumed periodic BC's. We thus have

$$e_0(\rho, v) \leq \lim_{\substack{L,N\to\infty \\ N/L^3 = \rho}} \frac{N(N-1)}{L^6} \int_{[0,L]^3} v(x) dx = \rho^2 \int_{\mathbb{R}^3} v(x) dx . \quad (21)$$

Usually one has $4\pi a < \int v(x) dx$. We are not quite there but close. As we will see one has to include a correlation factor in the wave function that reduces the probability for two particles to be close. This will allow us to obtain a better bound than (21) and to prove an upper bound of the form (8).

d.) The correct heuristics

Eq. (21) can be interpreted in the following way: In the dilute limit the probabity to find two particles in a region where they can interact is much larger than that a finding three particles in such a volume. Therefore the energy is given to leading order by $N(N-1)$ (number of pairs of particles) times the energy of a pair. In Eq. (21) this energy per pair was overestimated and given by $\int v(x)dx$.

The correct energy per pair is given by Eq. (5), that is, by $4\pi a$. It can be shown that the solution f of the scattering equation minimizes the energy $\mathcal{E}$ defined on p. 2. That is, f is the optimal shape of the wave function in the relative coordinate $r = x-y$ of a pair of particles with coordinates x and y that repel each other via v. This indicates that

$$\Psi(x_1 \ldots x_N) \sim \prod_{1 \le i < j \le N} f(x_i - x_j) \qquad (22)$$

might be a better trial state than Ψ_0.

e.) Why particles do not localize in order to minimize the interaction energy

One can ask the question why particles do not localize in different volumes s.t. their interaction energy vanishes. The answer is that this cannot happen because the resulting kinetic energy would be too large. From Eq. (8) we know that the energy per particle (not per volume) is given by $4\pi a\rho$. The related length scale ℓ_h called the healing length is given by

$$\ell_h = \sqrt{\frac{1}{4\pi\rho a}} \,. \tag{23}$$

It provides us with a length scale on which particles can be localized without causing the energy to explode. Since

$$a \ll \rho^{-1/3} \ll \ell_h \tag{24}$$

the particles cannot be localized such that their wave functions do not overlapp substantially.

After this heuristic discussion we start with the proof of the Theorem. We start with the upper bound.

3. The upper bound (Lieb, Seiringer, Yngvason 2000)
(In case of hard cores Dyson 1957)

We will prove the following upper bound for the energy on finite boxes.

<u>Theorem (Upper bound):</u> Let $\rho_1 = \frac{N-1}{L^3}$ and $b = (4\pi\rho_1/3)^{-1/3}$. For $b>a$ the ground state energy $E_0(N,L,V)$ with periodic boundary conditions satisfies

$$\frac{E_0(N,L,V)}{N} \leq 4\pi\rho_1 a \left(1+ \text{const.}\ \frac{a}{b}\right). \tag{25}$$

Thus in the thermodynamic limit (and for all boundary conditions)

$$\frac{e_0(\rho,V)}{4\pi a\rho^2} \leq 1+ \text{const.}\ Y^{1/3} \tag{26}$$

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

<u>Proof:</u> As we have already noted, the trial wave function need not be symmetric because this can only increase the energy. We choose a trial state of the form

$$\Psi(x_1 \ldots x_N) = F_1(x_1)\, F_2(x_1,x_2) \ldots F_N(x_1 \ldots x_N) \tag{27}$$

with $F_1 \equiv 1$ and where F_i depends only on the distance of

x_i to its nearest neighbor among the points $x_1, \dots, x_{i-1}$:

$$F_i(x_1 \dots x_i) = f(t_i) \quad \text{with} \quad t_i = \min\{|x_i - x_j|,\ j = 1 \dots i-1\}. \tag{28}$$

For f we make the choice

$$f(r) = \begin{cases} f_0(r)/f_0(b) & \text{for } 0 \le r \le b \\ 1 & \text{for } r > b \end{cases} \tag{29}$$

with $f_0(|x|)$ denoting the solution of the scattering equation. We note that $0 \le f(r) \le 1$ and $f'(r) \geq 0$ for all $r \geq 0$.

<u>Remark 1:</u> The function f defined in Eq. (29) minimizes the energy

$$\mathcal{E}_b(f) = \int_{B_b(0)} \{ |\nabla f(x)|^2 + \tfrac{1}{2} v(x) |f(x)|^2 \} dx \tag{30}$$

among all function in $H^1_1(B_b(0)) = \{ \psi = 1 + g \mid g \in H^1_0(B_b(0)) \}$.
Its energy is given by $4\pi a \left(1 - \frac{a}{b}\right)^{-1}$. (This follows from the computation on p. 2/3) $\quad (30^*)$

<u>Remark 2:</u> The trial state Ψ in Eq. (27) seems less natural than the one in Eq. (22) because it does not capture all correlations in the system. It is computationally easier to handle, however, and gives the correct leading order asymptotics.

We start by computing the kinetic energy of Ψ. Define

$$\varepsilon_{ik}(x_1 \dots x_N) = \begin{cases} 1 & \text{for } i=k \\ -1 & \text{for } t_i = |x_i - x_k| \\ 0 & \text{otherwise} \end{cases} \qquad (31)$$

and let n_i be the unit vector in the direction $x_i - x_{j(i)}$, where $x_{j(i)}$ denotes the nearest neighbor of x_i among the points $(x_1, \dots, x_{i-1})$. Although the notation indicates otherwise, $j(i)$ depends on all the points $x_1 \dots x_i$. Except for a set of zero measure $j(i)$ is well defined. Then

$$F^{-1} \nabla_k F = F^{-1} \nabla_k \prod_{i=1}^{N} f(t_i) = \sum_{i=1}^{N} F_i^{-1} \varepsilon_{ik} n_i f'(t_i). \qquad (32)$$

Next we compute

$$F^{-2} \sum_{k=1}^{N} |\nabla_k F|^2 = \sum_{i,j,k=1}^{N} F_i^{-1} F_j^{-1} \varepsilon_{ik} \varepsilon_{jk} (n_i \cdot n_j) f'(t_i) f'(t_j) \qquad (33)$$

$$\leq 2 \sum_{i=1}^{N} F_i^{-2} f'(t_i)^2 + 2 \sum_{k \leq i < j} |\varepsilon_{ik} \varepsilon_{jk}| \, F_i^{-1} F_j^{-1} f'(t_i) f'(t_j)$$

$i=j=k$ or $i=j\neq k$
and $t_i = |x_i - x_k|$

For the energy of our trial state this implies

Lemma: The function f_0 is monotone increasing, and hence $f_0'(r) \geq 0$.

$$\frac{\langle \Psi, H_N \Psi\rangle}{\langle \Psi,\Psi\rangle} \le 2\sum_{i=1}^{N} \frac{\int |\Psi(X)|^2 F_i^{-2}(x_1 \dots x_i)\, f'(t_i)^2\, dX}{\int |\Psi(X)|^2 dX} \tag{34}$$

(Note that Ψ is not normalized, and hence we need this factor)

$$+ \sum_{1\le i<j\le N} \frac{\int |\Psi(X)|^2\, v(x_i - x_j)\, dX}{\int |\Psi(X)|^2 dX}$$

$$+ 2\sum_{k\le i<j} \frac{\int |\Psi(X)|^2\, |\varepsilon_{ik}\varepsilon_{jk}|\, F_i(x_1 \dots x_i)^{-1} F_j(x_1 \dots x_j)^{-1} f'(t_i) f'(t_j)\, dX}{\int |\Psi(X)|^2 dX}$$

Let $i<p$ and define $F_{p,i}$ to be the value that F_p would take if the point x_i were omitted from consideration as a possible nearest neighbor. We note that $F_{p,i}$ does not depend on x_i! Analogously we define $F_{p,ij}$ by omitting x_i and x_j. In the following we will exploit cancellations between the numerators in (34) and the denominator. To that end, we first derive upper and lower bounds for F_i.

Since f is monotone increasing we have

$$F_p = \min\{ F_{p,ij},\, f(|x_p - x_i|),\, f(|x_p - x_j|)\}. \tag{35}$$

With $0 \le f \le 1$ we see that

$$F_{p,i,j}^2 \, f(|x_p - x_i|)^2 f(|x_p - x_j|)^2 \le F_p^2 \le F_{p,i,j}^2 . \qquad (36)$$

For $j<i$, we therefore have the upper bound

$$F_{j+1}^2 \cdots F_{i-1}^2 F_{i+1}^2 \cdots F_N^2 \le F_{j+1,ij}^2 \cdots F_{i-1,ij}^2 F_{i+1,ij}^2 \cdots F_{N,ij}^2 . \qquad (37)$$

To prove a lower bound, we need the following Lemma.

<u>Lemma:</u> Let $\{a_i\}_{i=1}^N$ be a sequence of real numbers with $0 \le a_i \le 1$ for all $i = 1 \ldots N$. Then

$$\prod_{i=1}^N (1 - a_i) \ge 1 - \sum_{i=1}^N a_i \qquad (38)$$

<u>Proof:</u> We write

$$\prod_{i=1}^N (1-a_i) = 1 - \sum_{i=1}^N a_i + \sum_{\substack{ij=1\\ i\neq j}}^N a_i a_j - \sum_{\substack{ijk=1\\ i\neq j\neq k\\ i\neq k}}^N a_i a_j a_k + \ldots + (-1)^N a_1 \ldots a_N \qquad (39)$$

$$= 1 - \sum_{i=1}^N a_i + \underbrace{\sum_{\substack{ij=1\\ i\neq j}}^N a_i a_j}_{\ge 0} \Bigg\{ 1 - \sum_{\substack{k=1\\ k\neq ij}}^N a_k + \sum_{\substack{kl=1\\ k\neq l\\ k,l\neq ij}}^N a_k a_l - \ldots + (-1)^{N-2} \prod_{\substack{k=1\\ k\neq ij}}^N a_k \Bigg\}$$

(*)

$$(*) = \prod_{\substack{k=1 \\ k \neq ij}}^{N} \left(1 - a_i\right) \geq 0.$$

$\blacksquare$

This proves the claim.

$$\prod_{k=1}^{j-1} f(|x_k - x_j|)^2 \prod_{q=1}^{i-1} f(|x_q - x_i|)^2$$

Using the Lemma, we show that

$$F_j^2 \dots F_N^2 \geq F_{j+1,ij}^2 \dots F_{i-1,j}^2 \, F_{i+1,ij}^2 \dots F_{N,ij}^2 \, f(|x_{j+1} - x_j|)^2 \dots f(|x_{i-1} - x_j|)^2$$

$$f(|x_{i+1} - x_i|)^2 f(|x_{i+1} - x_j|)^2 \dots f(|x_N - x_i|)^2 f(|x_N - x_j|)^2$$

$$\geq F_{j+1,ij}^2 \dots F_{i-1,j}^2 \, F_{i+1,ij}^2 \dots F_{N,ij}^2 \left(1 - \sum_{\substack{k=1 \\ k \neq ij}}^{N} \left(1 - f(|x_k - x_j|)^2\right)\right)$$

$$\left(1 - \sum_{\substack{k=1 \\ k \neq i}}^{N} \left(1 - f(|x_k - x_i|)\right)\right) \tag{40}$$

holds. Let us consider the first term on the right-hand side of (34) and use the bound

$$f'(t_i)^2 \leq \sum_{j=1}^{i-1} f'(x_i - x_j)^2. \tag{41}$$

We obtain

$$2 \sum_{i=1}^{N} \frac{\int |\Psi(X)|^2 \, F_i^{-2}(x_1 \dots x_i) \, f'(t_i)^2 \, dX}{\int |\Psi(X)|^2 dX} \leq$$

$$2\sum_{i=1}^{N}\sum_{j=1}^{i-1}\frac{\int |\Psi(X)|^2 F_i^{-2}(x_1\dots x_i)\, f'(x_i-x_j)^2\, dX}{\int |\Psi(X)|^2\, dX} \qquad (42)$$

To estimate the second term we use $F_j \le f(|x_i-x_j|)$ for $i<j$:

$$\sum_{1\le i<j\le N}\frac{\int |\Psi(X)|^2 v(x_i-x_j)\, dX}{\int |\Psi(X)|^2 dX} \qquad (43)$$

$$\le \sum_{1\le i<j\le N}\frac{\int F_1^2\dots F_{j-1}^2 f(|x_i-x_j|)^2 F_{j+1}^2\dots F_N^2\, v(x_i-x_j)\, dX}{\int F_1^2\dots F_N^2\, dX}$$

$$\overset{(37)}{\underset{(40)}{\le}} \sum_{1\le i<j\le N}\frac{\overbrace{\int F_1^2\dots F_{j-1}^2 f(|x_i-x_j|)^2 F_{j+1,j}^2 \dots F_{i-1,j}^2\, F_{i+1,ij}^2 \dots F_{N,ij}^2\, v(x_i-x_j)\, dX}^{(a)}}{\underbrace{\int F_1^2\dots F_{j-1}^2\, F_{j+1,j}^2 \dots F_{i-1,j}^2\, F_{i+1,ij}^2 \dots F_{N,ij}^2 \cdot (*)\, dX}_{(b)}}$$

$$(*) = \Big(1-\sum_{\substack{k=1\\k\ne j}}^{N}\big(1-f(|x_k-x_i|)^2\big)\Big)\Big(1-\sum_{\substack{k=1\\k\ne i,j}}^{N}\big(1-f(|x_k-x_j|)^2\big)\Big)$$

In the numerator we carry out the x_i and the x_j integration and find

$$(a) = \int F_1^2\dots F_{j-1}^2\, F_{j+1,j}^2\dots F_{i-1,j}^2\, F_{i+1,ij}^2\dots F_{N,ij}^2\, d(x_1\dots x_{i-1}x_{i+1}\dots x_{j-1}x_{j+1}\dots x_N)$$

$$\cdot \int v(x_i-x_j)\, f(|x_i-x_j|)^2\, d(x_i,x_j) \qquad (44)$$

To estimate (b) we use

$$\int \Big(1 - \sum_{\substack{k=1 \\ k \neq i}}^{N} \big(1 - f(|x_k - x_i|)^2 \big) \Big) dx_i \tag{45}$$

$$\geq L^3 - (N-1) \int \big(1 - f(|x|)^2 \big) dx$$

$$\left[\text{for } |x| \leq b \text{ use } f(x) \geq f_0(|x|)/f_0(b) \underset{\substack{(4),\ b > a \\ b > R_0}}{\geq} \frac{\left[1 - \frac{a}{|x|}\right]_+}{1 - \frac{a}{b}} \geq \left[1 - \frac{a}{|x|} \right]_+ \right]$$

$$\geq L^3 - (N-1) \underbrace{\int_{B_b(0)} \left(1 - \left[1 - \frac{a}{|x|} \right]_+^2 \right) dx}$$

$$= 4\pi \int_0^a r^2 dr + 4\pi \int_a^b \left(1 - \left(1 - \frac{2a}{r} + \frac{a^2}{r^2} \right) \right) r^2 dr$$

$$= 4\pi a^3/3 + 4\pi a (b^2 - a^2) - 4\pi a^2 (b-a)$$

$$= 4\pi a^3 \left(\tfrac{1}{3} - 1 + 1 \right) + 4\pi a b^2 - 4\pi a^2 b \leq 4\pi a b^2$$

$$\geq L^3 - (N-1) J \quad \text{with } J \leq 4\pi a b^2 .$$

From the x_j integration we obtain the same factor with $N-1$ replaced by $N-2$. Accordingly,

$$(b) \geq \int F_1^2 \dots F_{j-1}^2 \, F_{j+1,j}^2 \dots F_{i-1,j}^2 \, F_{i+1,ij}^2 \dots F_{N,ij}^2 \, d(x_1 \dots x_{i-1} x_{i+1} \dots x_{j-1} x_{j+1} \dots x_N)$$

$$\cdot \left(L^3 - (N-1) J \right)^2 \quad \text{with} \quad J \leq 4\pi a b^2. \tag{46}$$

The bounds for (a) and (b) imply that the second term on the right-hand side of (34) is bounded from above by

$$N(N-1) \frac{\int v(x-y) f(x-y)^2 \, d(x,y)}{\left(L^3 - (N-1) J \right)^2} . \tag{47}$$

Using (42), we also see that the first term on the right-hand side of (34) is bounded from above by

$$2 \sum_{i=1}^{N} \sum_{j=1}^{i-1} \frac{\int f'(x_i - x_j)^2 \, d(x_i, x_j)}{\left(L^3 - (N-1) J \right)^2} = \frac{2N(N-1) L^3 \int_{[0,L]^3} f'(x)^2 dx}{\left(L^3 - (N-1) J \right)^2}. \tag{48}$$

The sum of (47) and (48) is given by $\left(L > 2b \right)$

$$\frac{N(N-1) L^3}{\left(L^3 - (N-1) J \right)^2} \int_{\mathbb{R}^3} \left\{ f'(x)^2 + \tfrac{1}{2} v(x) f(x)^2 \right\} dx \overset{(29),(30^*)}{=} \frac{N(N-1) L^3 \, 4\pi a}{\underbrace{\left(L^3 - (N-1) 4\pi a b^2 \right)^2}\left(1 - \frac{a}{b} \right)} \tag{49}$$

$$= L^3 \Big(1 - \underbrace{\frac{N-1}{L^3}}_{\rho_1} 4\pi a b^2 \Big)$$

$$\leq \frac{N(N-1)}{L^3} 4\pi a \left(1+O\left(a/b\right)\right)$$ if we assume that $b\varrho^{1/3} \leq$ const. holds for $\varrho^{1/3}a \to 0$. The optimal choice for b is thus proportional to $\varrho^{-1/3}$.

Exercise 2: Use the above techniques to show that the third term on the right-hand side of (34) is bounded from above by

$$\frac{3}{2} N(N-1)(N-2) \frac{K^2}{\left(L^3-(N-1)J\right)^2}, \tag{50}$$

where $K = \int f(x) f'(x) dx$. Use $\left[1-\frac{a}{|x|}\right]_+ \leq f(x) \leq 1$ and partial integration to show that

$$K \leq 4\pi a b\left(1+O(a/b)\right) \tag{51}$$

holds.

In combination, (50) and (51) imply that the third term on the right-hand side of (34) is for bounded ϱb^3 bounded from above by a constant times

$$N a^2 \varrho_1 / b. \tag{52}$$

We use (52) and (49) to prove (25) and (26) (up to constant factors that are supposedly not correct in the Theorem). $\boxed{\text{YL}}$

Exercise 3: Use the trial state $\Psi(x_1 \ldots x_N) = \dfrac{\prod_{1 \le i < j \le N} f(x_i - x_j)}{\left\| \prod_{1 \le i < j \le N} f(x_i - x_j) \right\|}$ and

try for a short while to obtain cancellations in the numerator and the denominator of the expectation of the energy $\langle \Psi, H_N \Psi \rangle$. Afterwards you will most likely appreciate the computations on the previous pages more than before.

Exercise 4: Use the trial state Ψ from above and prove an estimate for the energy in finite boxes without taking cancellations between the numerator and the denominator into account. Use $f(x) \le 1$ in the numerator and the Lemma on p. 17 in the denominator whenever you can. If you have the bound consider the combined thermodynamic and low density limit $N \to \infty$, $L \to \infty$, $N/L^3 = \rho =$ fixed and $a = a_N = \frac{a_0}{N}$ with a_0 fixed. Can you prove the equivalent of (8) in this limit?

4. The lower bound (Lieb, Yngvason 1998)

In this Section we are going to prove the following Theorem:

<u>Theorem</u> (<u>Lower bound in a finite box</u>): For every interaction potential v (as in the Theorem on p.4) there is a $\delta > 0$ such that the ground state energy of H_N with Neumann boundary conditions satisfies

$$\frac{E_0(N,L,v)}{N} \geq 4\pi a\varrho\left(1 - CY^{1/17}\right) \qquad (53)$$

for all N and L with $Y < \delta$ and $L/a > C'Y^{-6/17}$. Here C and C' are positive constants, independent of N and L.

<u>Remark</u>: The above Theorem implies the lower bound we are looking for in the thermodynamic limit.

<u>Main idea</u>: As the discussion before the proof of the upper bound indicates the energy looks like first order perturbation theory

$$\left[\begin{array}{l} H(\lambda) = H_0 + \lambda H_1 \,;\; H_0\Psi_0 = E_0\Psi_0 \,;\; H(\lambda)\Psi(\lambda) = E(\lambda)\Psi(\lambda) \\ \quad \Rightarrow\; E(\lambda) = E_0 + \lambda\langle\Psi_0, H_1\Psi_0\rangle + o(\lambda) \end{array}\right] \qquad (54)$$

with the notable difference that the interaction potential is so singular that additional correlation have to be taken into account. Because of these correlation the energy is a sum of kinetic and potential energy and not just potential energy alone.

To take the above into accound we first use some part of the kinetic energy to replace the original interaction potential by a softer one with longer range. To this potential we will then apply a rigorous version of first order perturbation theory (Temples inequality).

Proof: We start with a Lemma that allows us to replace the interaction potential in the way we just explained.

Lemma (Dyson Lemma): Let $v(r) \geq 0$ with finite range R_0.

Let $U: \mathbb{R}_+ \to \mathbb{R}_+$ be any function satisfying $\int_0^\infty U(r) r^2 dr \leq 1$ and $U(r) = 0$ for $r < R_0$. Let $B \subset \mathbb{R}^3$ be star shaped with respect to 0. Then for all differentiable functions Ψ

$$\int_B \left(|\nabla \Psi(x)|^2 + \tfrac{1}{2} v(x) |\Psi(x)|^2 \right) dx \geq a \int_B U(|x|) \, |\Psi(x)|^2 dx, \qquad (55)$$

where a denotes the scattering length of v.

Proof: As we will see, the inequality holds with $|\nabla \Psi(x)|^2$ replaced by $\left|\frac{\partial \Psi(x)}{\partial r}\right|^2$ (the radial part of the kinetic energy, $\int |\nabla \Psi(x)|^2 dx \geq \int \left|\frac{\partial \Psi}{\partial r}(x)\right|^2 dx$). Accordingly, it suffices to prove (55) on a line segment with fixed angular variables. We write $\Psi(x) = \tilde{\Psi}(r,\omega)$ and need to show that

Could be $+\infty$.

$$\int_0^{R_1} \left\{ \left| \frac{\partial \tilde{\Psi}(r,\omega)}{\partial r} \right|^2 + \tfrac{1}{2} V(r) \left| \tilde{\Psi}(r,\omega) \right|^2 \right\} r^2 dr \geq a \int_0^{R_1} \mathcal{U}(r) r^2 \left| \tilde{\Psi}(r,\omega) \right|^2 dr \quad (56)$$

holds. We will prove (56) first for the choice $\mathcal{U}(r) = \frac{1}{R^2} \delta(r-R)$ with $R > R_0$ and then reduce the general case to this case. The right-hand side of (56) with this choice reads

$$a \int_0^{R_1} \frac{1}{R^2} \delta(r-R) r^2 \left| \tilde{\Psi}(r,\omega) \right|^2 dr = \begin{cases} 0 & \text{if } R > R_1 \\ a |\tilde{\Psi}(R,\omega)|^2 & \text{if } R \leq R_1 . \end{cases} \quad (57)$$

For $R > R_1$ the inequality is trivial because $V \geq 0$. In the other case we use (30*) as well as the fact that the minimizer of (30) is a radial function to see that

$$\int_0^{R_1} \left\{ \left| \frac{\partial \tilde{\Psi}(r,\omega)}{\partial r} \right|^2 + \tfrac{1}{2} V(r) \left| \tilde{\Psi}(r,\omega) \right|^2 \right\} r^2 dr \geq \frac{a}{1 - \frac{a}{R}} \left| \tilde{\Psi}(R,\omega) \right|^2 \quad (58)$$

$$\overset{a \leq R_0 < R}{\geq} a \left| \tilde{\Psi}(R,\omega) \right|^2$$

holds. To obtain this result, we used $R > R_0$. This proves (56) for $\mathcal{U}(r) = \frac{1}{R^2} \delta(r-R)$. Next we integrate (58) against the measure $\mathcal{U}(R) R^2 dR$ and find

$$\underbrace{\int_0^\infty \mathcal{U}(R)R^2\,dR}_{\leq 1} \int_0^{R_1} \left\{ \left| \frac{\partial \tilde{\Psi}(r,\omega)}{\partial r} \right|^2 + \tfrac{1}{2} v(r) \left| \tilde{\Psi}(r,\omega) \right|^2 \right\} r^2\,dr \tag{59}$$

$$\geq a \int_0^\infty \mathcal{U}(R) R^2 \left| \tilde{\Psi}(R,\omega) \right|^2 dR .$$

Finally, we integrate ω over S^2 and obtain

$$\int_{\mathbb{R}^3} \left\{ \left| \frac{\partial \Psi(x)}{\partial r} \right|^2 + \tfrac{1}{2} v(x) |\Psi(x)|^2 \right\} dx \geq a \int_{\mathbb{R}^3} \mathcal{U}(|x|) |\Psi(x)|^2 dx . \tag{60}$$

Since $\int_{\mathbb{R}^3} |\nabla \Psi(x)|^2 dx \geq \int_{\mathbb{R}^3} \left| \frac{\partial \Psi(x)}{\partial r} \right|^2 dx$ (Check!), this proves the claim.

$\boxtimes$

<u>Corollary 1:</u> For any function $\mathcal{U}$ as in the Dyson Lemma we have

$$H_N \geq a W \tag{61}$$

with the multiplication operator

$$W(x_1 \dots x_N) = \sum_{i=1}^N \mathcal{U}(t_i), \tag{62}$$

where t_i is the distance of x_i to its nearest neighbor, that is,

$$t_i(x_1 \ldots x_N) = \min_{\substack{j=1\ldots N \\ j \neq i}} |x_i - x_j|. \tag{63}$$

Remark: Note that t has a different meaning than in the proof of the upper bound.

Proof: For given points $x_1 \ldots x_N$ we divide $[0,L]^3$ into Voronoi cells B_i that contain all points closer to x_i than to x_j with $j = 1 \ldots N$, $j \neq i$.

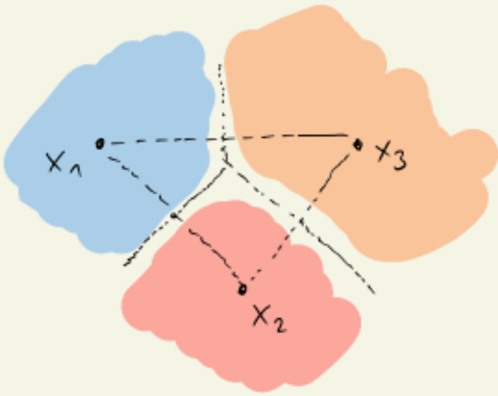

Fig 1: Example of Voronoi cells.

One easily checks that Voronoi cells are convex and therefore star shaped. To obtain (61) we drop all interactions except for next neighbor interactions for a lower bound and apply the Dyson Lemma in the Voronoi cells B_i.

$\blacksquare$

For the potential $\mathcal{U}$ we make the choice

$$\mathcal{U}_R(r) = \begin{cases} 3\,(R^3 - R_0^3)^{-1} & \text{for } R_0 < r < R, \\ 0 & \text{otherwise.} \end{cases} \tag{64}$$

The corresponding N-particle interaction will be denoted by W_R.

Next, we choose $\varepsilon > 0$ and write

$$H_N = \varepsilon H_N + (1-\varepsilon) H_N \geq \varepsilon \underbrace{\sum_{i=1}^{N} -\Delta_i}_{T_N} + (1-\varepsilon) H_N . \tag{65}$$

In combination with Corollary 1, this gives

$$H_N \geq \varepsilon T_N + (1-\varepsilon)\, a\, W_R . \tag{66}$$

We consider the operator on the right-hand side from the viewpoint of first order perturbation theory, with εT_N as the unperturbed part denoted by H_0. To that end, we first prove the following Lemma.

<u>Lemma (Temple's inequality)</u>: Let H_0 be as above and let $V \in L^2([0,L]^{3N})$. Let $E_0 < E_1$ be the two smallest eigenvalues of $H = H_0 + V$ and let Ψ_0 be the unique ground state of H_0, that is, $H_0 \Psi_0 = 0$. Then

$$E_0 \geq \langle \Psi_0, H\Psi_0\rangle - \frac{\langle \Psi_0, H^2\Psi_0\rangle - \langle \Psi_0, H\Psi_0\rangle^2}{E_1 - \langle \Psi_0, H\Psi_0\rangle} \qquad (67)$$

provided $E_1 - \langle \Psi_0, H\Psi_0\rangle > 0$. If in addition $V \geq 0$, then we can replace E_1 on the right-hand side of (67) by $E_1^{(0)}$, the second lowest eigenvalue of H_0.

Proof: We start by noting that

$$(H - E_0)(H - E_1) \geq 0 \qquad (68)$$

$$\Leftrightarrow \quad H^2 + E_0 E_1 - E_0 H - E_1 H \geq 0$$

$$\Rightarrow \quad \langle \Psi_0, H^2\Psi_0\rangle + E_0E_1 - (E_0 + E_1)\langle \Psi_0, H\Psi_0\rangle \geq 0$$

$$\Rightarrow \quad E_0\left(E_1 - \langle \Psi_0, H\Psi_0\rangle\right) \geq -\langle \Psi_0, H^2\Psi_0\rangle + E_0\langle \Psi_0, H\Psi_0\rangle.$$

We divide by $E_1 - \langle \Psi_0, H\Psi_0\rangle$ to show (67). The second claim follows from the min-max principle for the eigenvalues of H (see the last Theorem in the introduction).

$\blacksquare$

We apply Temple's inequality with the choice $H_0 = \varepsilon T_N$ and $H = H_0 + (1-\varepsilon) a W_R$. In this case $\Psi_0(x_1 \dots x_N) = \left(L^{-3/2}\right)^N$. There are several quantities we need to compute (or estimate) and we start with $\langle \Psi_0, H \Psi_0 \rangle = (1-\varepsilon)\, a \, \langle \Psi_0, W_N \Psi_0 \rangle$. We claim that

$$4\pi\rho\left(1-\frac{1}{N}\right) \geq \frac{\langle \Psi_0, W_R \Psi_0 \rangle}{N} \geq 4\pi\rho\left(1-\frac{1}{N}\right)\left(1-\frac{2R}{L}\right)^3\left(1-\frac{4\pi}{3}\rho R^3\right) \qquad (69)$$

We start by proving the lower bound:

$$\langle \Psi_0, W_N \Psi_0 \rangle = \frac{1}{L^{3N}} \sum_{i=1}^{N} \int_{[0,L]^{3N}} \mathcal{U}(t_i)\, d(x_1 \ldots x_N) \qquad (70)$$

Symmetry + Definition of $\mathcal{U}(t_i)$

$$= \frac{N}{L^{3N}} \frac{3}{R^3 - R_0^3} \int_{[0,L]^{3N}} \mathbb{1}\left(R_0 < t_1 < R\right) d(x_1 \ldots x_N)$$

$$\geq \frac{N}{L^{3N}} \frac{3}{R^3 - R_0^3} \int_{[R, L-R]^3 \times [0,L]^{3(N-1)}} \mathbb{1}\left(R_0 < t_1 < R\right) d(x_1 \ldots x_N)$$

The smaller cube is introduced to avoid boundary effects for the coordinates $x_2 \ldots x_N$ when they interact with x_1.

We obtain a lower bound for the above integral if we assume that for fixed x_1, only one coordinate out of $x_2 \dots x_N$ is an element of the set $\{ x \in [0,L]^3 \mid R_0 < |x_1 - x| < R \}$ and the other coordinates are in $x \in [0,L]^3 \setminus \{ |x| > R \}$. Note that there are $N-1$ such terms because each x_i, $i = 2 \dots N$ interacts with x_1. We find

$$\frac{\langle \Psi_0, W_R \Psi_0 \rangle}{N} \geq \frac{3N(N-1)}{(R^3 - R_0^3)N} \frac{(L-2R)^3}{L^3} \frac{4\pi}{3} \frac{R^3 - R_0^3}{L^3} \left(\frac{L^3 - \frac{4\pi}{3} R^3}{L^3} \right)^{N-2}$$

$$= 4\pi \rho \left(1 - \frac{1}{N}\right)\left(1 - \frac{2R}{L}\right)^3 \left(1 - \frac{4\pi}{3}\frac{R^3}{L^3}\right)^{N-2} \tag{71}$$

$$\overset{(38)}{\geq} 4\pi \rho \left(1 - \frac{1}{N}\right)\left(1 - \frac{2R}{L}\right)^3 \left(1 - \frac{4\pi}{3} \rho R^3\right).$$

This proves the claimed lower bound. For the upper bound we argue similarly and realize that if $x_i \in \{ x \in [0,L]^3 \mid R_0 < |x_1 - x| < R \}$, $i = 2 \dots N$, then we obtain an upper bound if we estimate the integral over all other coordinates by 1. Hence,

$$\langle \Psi_0, W_N \Psi_0 \rangle \leq \frac{N(N-1)}{L^6} \frac{3}{R^3 - R_0^3} \int_{[0,L]^6} \mathbb{1}\left(R_0 < |x_1 - x_2| < R \right) d(x_1, x_2)$$

$$\leq \frac{N(N-1)}{L^3} 4\pi = \frac{4\pi N^2}{L^3}\left(1 - \frac{1}{N}\right), \tag{72}$$

which proves the claimed upper bound.

Next we insert into the lower bound that we obtain from Temple's inequality. This gives

$$\frac{E_0}{N} \geq 4\pi a \rho \left(1-\varepsilon\right)\left(1-\frac{1}{N}\right)\left(1-\frac{2R}{L}\right)^3\left(1-\frac{4\pi}{3}\rho R^3\right) \qquad (73)$$

$$\left(1 - \frac{a\left(\langle \Psi_0, W_R^2 \Psi_0\rangle - \langle \Psi_0, W_R \Psi_0\rangle^2\right)}{\langle \Psi_0, W_R \Psi_0\rangle \left(E_1^{(0)} - a\langle \Psi_0, W_R \Psi_0\rangle\right.}\right)$$

$$= 4\pi a \rho \left(1 - \mathcal{E}(\rho, L, R, \varepsilon)\right). \quad \left(\text{Defining equation for } \mathcal{E}(\rho, L, R, \varepsilon)\right)$$

To estimate $\langle \Psi_0, W_R^2 \Psi_0\rangle$ from above we realize that $\mathcal{U}_R^2 = \frac{3}{R^3 - R_0^3}\mathcal{U}_R$.
Using this bound, we estimate

$$\langle \Psi_0, W_R^2 \Psi_0\rangle = \sum_{i,j=1}^{N} \langle \Psi_0, \underbrace{\mathcal{U}(t_i)\mathcal{U}(t_j)}_{\substack{\leq \frac{1}{2}\mathcal{U}(t_i)^2 + \frac{1}{2}\mathcal{U}(t_j)^2 \\ \leq \frac{1}{2}\frac{3}{R^3 - R_0^3}\left(\mathcal{U}(t_i) + \mathcal{U}(t_j)\right)}} \Psi_0\rangle \leq \frac{3N}{R^3 - R_0^3}\langle \Psi_0, W_R \Psi_0\rangle. \qquad (74)$$

We also note that $E_1^{(0)} = \frac{\pi^2}{L^2}$ (Check! Compute second eigenvalue of the Neumann Laplacian in $[0,L]^3$).

At this point we should notice that we cannot take the thermodynamic limit on both sides of (73). This is because $E_1^{(0)} - a\langle \Psi_0, W_R \Psi_0\rangle$ behaves as $\varepsilon L^{-2} - a\rho^2 L^3$ (we ignore constants and subleading corrections). For L large enough this term becomes negative and Temple's inequality looses its validity.

To avoid this problem we divide the box $[0,L]^3$ into smaller boxes with side length l that is kept fixed as $L \to \infty$. The number L/l of small boxes will increase. The N particles are distributed among the smaller boxes, and we use (73), with L replaced by l, N replaced by the particle number n in a small box (which might vary from box to box) and ρ replaced by n/l^3, to estimate the energy in each box with Neumann boundary conditions. For each distribution of the N particles over the L/l boxes we add up the contributions from the small boxes by neglecting interactions between particles in different boxes. Since $V \geq 0$ this can only lower the energy. Finally, we minimize over all possible configurations of the particles. The energy we obtain like this is a lower bound to $E_0(N,L)$, because by separating space into smaller boxes with Neumann boundary conditions we effectively allow for test functions, which are less regular than the ones in the form domain of H_N. We find

$$\frac{E(N,L)}{N} \geq \left(\rho\ell^3\right)^{-1} \inf_{\substack{\sum_{n\geq 0} c_n = 1 \\ \sum_{n\geq 0} c_n n = \rho \ell^3}} \sum_{n\geq 0} c_n E_0(n,\ell). \qquad (75)$$

Unfortunately, we do not know that $E_0(n,\ell)$ is convex (such a result only holds for the energy in the thermodynamic limit), because this would allow us to show that we have the same particle number in each box. We however know that the energy is superadditive. More precisely, because $V \geq 0$ we have

$$E_0(n+n',\ell) \geq E_0(n,\ell) + E_0(n,\ell). \qquad (\text{Check!}) \qquad (76)$$

Let $n,p \in \mathbb{N}$ with $n \geq p$ and denote by $[x]$ the largest integer smaller than x. Eq. (76) implies

$$E_0(n,\ell) \geq \left[\frac{n}{p}\right] E_0(p,\ell) \geq \frac{n}{2p} E_0(p,\ell). \qquad (77)$$

We replace N by n, L by ℓ and ρ by n/ℓ^3 in (73) and obtain for fixed R and ε

$$E_0(n,\ell) \geq \frac{4\pi a}{\ell^3} n(n-1) K(n,\ell) \tag{78}$$

with a function $K(n,\ell)$ determined by (73). We will later see that the map $n \mapsto K(n,\ell)$ is monotonously decreasing. For $p \in \mathbb{N}$ with $n \leq p$ we thus have

$$E_0(n,\ell) \geq \frac{4\pi a}{\ell^3} n(n-1)\, K(p,\ell). \tag{79}$$

For fixed p we now write

$$\sum_{n\geq 0} c_n E_0(n,\ell) = \sum_{0\leq n<p} c_n \underbrace{E_0(n,\ell)}_{\substack{(79)\\ \geq \frac{4\pi a}{\ell^3} n(n-1) K(p,\ell)}} + \underbrace{\sum_{n\geq p} c_n E_0(n,\ell)}_{(79),(77)}$$

$$\sum_{n\geq p} c_n E_0(n,\ell) \geq \frac{4\pi a}{\ell^3} p(p-1) K(p,\ell) + \sum_{n>p} \frac{n}{2p} \underbrace{E_0(p,\ell)}_{\geq \frac{4\pi a}{\ell^3} p(p-1) K(p,\ell)}$$

$$\geq \frac{4\pi a}{\ell^3} K(p,\ell) \left[\sum_{0\leq n<p} c_n\, n(n-1) + \sum_{n\geq p} c_n \frac{n(p-1)}{2} \right]. \tag{80}$$

It remains to minimize the right-hand side of (80) over $\{c_n\}_{n=0}^{\infty}$ w.r.t. the constraints $\sum_{n\geq 0} c_n = 1$ and $\sum_{n \geq 0} c_n n = \rho \ell^3$. Define

$$k := \rho \ell^3 \quad \text{and} \quad t := \sum_{n<p} c_n n \leq k \tag{81}$$

and note that $\sum_{n \geq p} c_n n = k - t$. We thus have

$$\inf_{\substack{\sum_{n\geq 0} c_n = 1 \\ \sum_{n\geq 0} c_n n = k}} \left\{ \underbrace{\sum_{n<p} c_n n(n-1)} + \underbrace{\frac{1}{2} \sum_{n\geq p} c_n n (p-1)}_{= \frac{p-1}{2}(k-t)} \right\} \tag{82}$$

$$\underbrace{\sum_{n<p} c_n n(n-1)} = \frac{1}{\sum_{n<p} c_n} \sum_{n<p} c_n \underbrace{n(n-1)}_{f(n)} \sum_{n<p} c_n$$

Convexity of $n \mapsto n(n-1)$ + Jensen's ineq.

$$\geq f\Bigg(\frac{1}{\underbrace{\sum_{n<p} c_n}_{\eta^{-1}}} \underbrace{\sum_{n<p} c_n n}_{t} \Bigg) \underbrace{\sum_{n<p} c_n}_{0 \leq \eta \leq 1}$$

$$= \frac{t}{\eta}\left(\frac{t}{\eta} - 1\right)\eta \geq t(t-1)$$

$$\geq \inf_{\substack{\sum_{n\geq 0} c_n = 1 \\ \sum_{n\geq 0} c_n n = k}} \left\{ t(t-1) + \frac{1}{2}(p-1)(k-t) \right\}$$

We have to minimize the expression in the brackets for $0 \leq t \leq k$. If $p \geq 4k$ the minimum is taken at $t = k$ and equals $k(k-1)$. We choose $p = 4k = 4\rho\ell^3$ and find with (75) and (80)–(82) that

$$\frac{E_0(N,L)}{N} \geq 4\pi a\rho \overset{(*)}{\left(1 - \frac{1}{\rho\ell^3}\right)} K(4\rho\ell^3, \ell) \qquad (83)$$

holds. Using (69), (73), (74) and (78), we see that the function K can be chosen as

$$\tilde{K}(n,\ell) = (1-\varepsilon)\left(1 - \frac{2R}{\ell}\right)^3\left(1 - \frac{4\pi}{3}\rho R^3\right) \qquad (84)$$

$$\times \left(1 - \underbrace{\frac{a\left(\langle\psi_0, w_R^2\psi_0\rangle - \langle\psi_0, w_R\psi_0\rangle^2\right)}{\langle\psi_0, w_R\psi_0\rangle\left(E_1^{(0)} - a\langle\psi_0, w_R\psi_0\rangle\right)}}_{\leq \frac{a\langle\psi_0, w_R\psi_0\rangle \frac{3n}{R^3 - R_0^3}}{\langle\psi_0, w_R\psi_0\rangle\left(\pi\varepsilon\ell^{-2} - 4\pi a\ell^{-3}n(n-1)\right)}}\right)$$

This is what we get if we look for the largest K satisfying (78) (given (73)).

$$\geq (1-\varepsilon)\left(1 - \frac{2R}{\ell}\right)^3\left(1 - \frac{4\pi}{3}\rho R^3\right)$$

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

This is a convenient choice for K.

The estimate (78) is valid as long as the denominator in the last factor is nonnegative. To obtain a bound for all u will use the trivial bound zero if the above is not satisfied. Note that $K(u,\ell)$ is a monotoneously decreasing function of u.

We insert $u = 4\rho\ell^3$ in the formula for K and obtain

$$K(4\rho\ell^3, \ell) \geq (1-\varepsilon)\left(1 - \frac{2R}{\ell}\right)^3 \left(1 - \text{const.}\,(a^3\rho)\,(\ell/a)^3\,(R/\ell)^3\right)$$
$$\times\left(1 - \frac{\ell^3}{R^3 - R_0^3}\;\frac{\text{const.}\; a^3\rho}{\varepsilon\,(a/\ell)^2 - \text{const.}\,(a^3\rho)\,(\ell/a)^3}\right). \tag{85}$$

For the parameters we make the ansatz

$$\varepsilon \sim (a^3\rho)^\alpha, \quad a/\ell \sim (a^3\rho)^\beta, \quad (R^3 - R_0^3)/\ell^3 \sim (a^3\rho)^\gamma. \tag{86}$$

We have the following requirements:

- $\varepsilon(a/\ell)^2 - \text{const.}\,(a^3\rho)(\ell/a)^3 > 0$. This holds for $a^3\rho$ small enough provided $\alpha + 5\beta < 2$.
- $\alpha > 0$ in order that $\varepsilon \to 0$ for $a^3\rho \to 0$.
- $3\beta - 1 > 0$ in order that $\frac{1}{a^3\rho}\left(\frac{a}{\ell}\right)^3 \to 0$ for $a^3\rho \to 0$, which is required to have $(*) \to 1$, see (83).

- $1-3\beta+\gamma>0$ in order that $(a^3\varrho)(\ell/a)^3\,\frac{R^3-R_0^3}{\ell^3}\to 0$ for $a^3\varrho\to 0$.

- $1-\alpha-2\beta-\gamma>0$ to control the last factor in (86).

The optimal choice for α,β,γ satisfying the constraints is

$$\alpha=\frac{1}{17},\quad \beta=\frac{6}{17},\quad \gamma=\frac{3}{17}. \tag{87}$$

This choice satisfies

$$\alpha=3\beta-1=1-3\beta+\gamma=1-\alpha-2\beta-\gamma=\frac{1}{17} \tag{88}$$

and allows us to finish the proof of (53). In combination with (25), (53) proves (8).

$\boxtimes$