ON THE EXCESS CHARGE PROBLEM OF ATOMS

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ABSTRACT. This paper establishes new bounds on the maximum number of electrons $N_c(Z)$ that an atom with nuclear charge Z can bind. Specifically, we show that

$$N_c(Z) < 1.1185Z + O(Z^{1/3})$$

with an explicit bound on the lower order term $O(Z^{1/3})$. This result improves long–standing bounds by Lieb and Nam obtained in 1984, respectively 2012. Our bounds show the fundamental difference between fermionic and bosonic atoms for finite Z since for bosonic atoms it is known that $\lim N_c(Z)/Z = t_c \approx 1.21$ in the limit of large nuclear charges Z.

CONTENTS

1.	Introduction	1
2.	Basic notation and main result	2
3.	The Benguria–Lieb–Nam Argument: Playing with weights	5
4.	Symmetry of minimizing sequences	9
5.	Mean-Field type bounds	17
6.	Upper bounds on the weighted kinetic energy	30
7.	Bounds on maximal excess charge	34
Appendix A. Technical Details		40
References		49

1. Introduction

It is widely accepted that a single atom in a vacuum can bind at most one or two additional electrons. From a heuristic perspective, this is evident: atoms are electrically neutral, and while an additional electron may coexist with the atom, the addition of more electrons becomes challenging due to Coulomb repulsion caused by the net-negative charge of the resulting configuration. Deriving this behavior from the many-body Schrödinger equation remains a challenging open question for many decades, [Sim84, Simoo].

An atom of nuclear charge Z should be able to bind at least N < Z+1 electrons, since the farthest out electron will experience a net Coulomb attraction to the nucleus, the remaining N-1 electrons cannot fully screen the charge of the nucleus when N-1 < Z. This was made rigorous in the early work of Zhislin [vZ69], so $\lim \inf_{Z \to \infty} \frac{N_c(Z)}{Z} \ge 1$ was known for a long time, already. That there is a critical number $N_c(Z) < \infty$ that an atom of charge Z

1

Key words and phrases. Many-Particle Schrödinger Operator, Ionization Conjecture, Atoms.

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can bind was first shown independently by Ruskai [Rus82] and Sigal [Sig82]. Later, Lieb, Sigal, Simon, and Thirring [LSST88] proved

$$\lim_{Z\to\infty}\frac{N_c(Z)}{Z}=1.$$

In fact, they proved the result with lim replaced by lim sup. That $N_c(Z) \ge Z$ was shown by Zhislin [Zhi6o] much earlier. The result by Lieb, Sigal, Simon and Thirring uses a compactness argument and does not provide any quantitative bounds on how big $N_c(Z)$ is for finite nuclear charge Z. Fefferman and Seco [FS90] and Seco, Sigal and Solovej [SSS90] proved in 1990

$$N_c(Z) \le Z + O(Z^{5/7})$$
 as $Z \to \infty$.

Non-asymptotic bounds are rare, for a long time the only non-asymptotic bound was due to Lieb [Lie84] who proved the famous bound

$$N_c(Z) < 2Z + 1$$
 for all $Z \ge 1$.

Lieb's result is independent of the statistic of the particles, i.e., independent of whether they are fermions of bosons, and it also holds, suitably modified, for systems of atoms, i.e., molecules. While Lieb's bound certainly overcounts $N_c(Z)$, it shows that Hydrogen (Z=1) can bind only two electrons, which is observed in nature.

It took 28 years until Nam's breakthrough result [Nam12] could significantly improve Lieb's longstanding bound. Nam showed for a single atom with fermionic statistics that

$$N_c(Z) < 1.22Z + 3Z^{1/3}$$
 for all $Z \ge 1$.

In this work, we provide even tighter bounds on N_c . In particular, we prove

$$N_c(Z) < 1.1185Z + 4Z^{1/3}$$
 for all $Z \ge 4$.

We would like to stress that this shows that for large nuclear charges Z fermionic atoms do indeed behave much differently from bosonic atoms. Bosonic atoms are known to allow for a surcharge of 21 %, i.e., large bosonic atoms can bind roughly $N \sim 1.21Z$ bosonic particles for large Z. The leading order coefficient in Nam's bound is just above 1.21 whereas in our bound it is lower, with a good safety margin.

To achieve our improvements, we significantly extend Nam's approach and, in addition, prove some of the conjectures made in [Nam12].

Acknowledgements: The authors wish to thank Ioannis Anapolitanos, Leonid Chaichenets, and Peer Kunstmann for insightful discussions, which greatly contributed to the development and refinement of this manuscript. Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 258734477 – SFB 1173.

2. Basic notation and main result

We consider a nucleus of charge Z placed at the origin and N particles located at positions $x_1, \dots x_N \in \mathbb{R}^3$. In the limit of infinite nuclear mass and after appropriate rescaling the

Schrödinger operator of a single atom is given by

$$H_{N,Z} := \frac{1}{2} \sum_{k=1}^{N} P_k^2 - \sum_{i=1}^{N} \frac{Z\alpha}{|x_i|} + \sum_{1 \le i < j \le N} \frac{\alpha}{|x_i - x_j|}.$$
 (2.1)

Here $\alpha = e^2/(\hbar c)$ is the fine structure constant and $P_j = -i\hbar \nabla_j$ denotes the usual three-dimensional momentum operator with respect to the variable x_j .

Remark 2.1. We choose atomic units, that is $\hbar = m_e = c = e = 1$ and consequently $\alpha = 1$. Another usual choice of units is setting the electron mass $m_e = 1/2$ as for example in [Lie76], such that the factor in the kinetic energy vanishes. The question on the maximal excess charge is independent of the choice of these units.

The Hilbert space of N particles of spin $S \in \mathbb{N}_0/2$ is the N-fold tensor product

$$\mathcal{H}_N := \bigotimes_{i=1}^N L^2(\mathbb{R}^3; \mathbb{C}^{2S+1}). \tag{2.2}$$

Let $z_1, ... z_N$ be the combined position–spin coordinate of a single particle, $z_j = (x_j, s_j)$. Considering identical particles we only consider stats $\psi \in \mathcal{H}_N$ such that

$$\left|\psi(\ldots z_i,\ldots,z_j,\ldots)\right|^2 = \left|\psi(\ldots z_j,\ldots,z_i,\ldots)\right|^2. \tag{2.3}$$

We distinguish between fermions or bosons. For fermions, the state space is the subspace of totally antisymmetric functions \mathcal{H}_N^f . We call $\psi \in \mathcal{H}_N$ totally antisymmetric if

$$\psi(\ldots z_i,\ldots,z_j,\ldots) = -\psi(\ldots z_j,\ldots,z_i,\ldots)$$
 for all $i \neq j \in \{1,\ldots,N\}$.

For bosons, we consider the subspace of totally symmetric functions denoted by \mathcal{H}_N^b . We call $\psi \in \mathcal{H}_N$ totally symmetric if

$$\psi(\ldots z_i,\ldots,z_j,\ldots)=\psi(\ldots z_j,\ldots,z_i,\ldots)$$
 for all $i\neq j\in\{1,\ldots,N\}$.

With regards to real atoms, the particles of interest are electrons and thus the fermionic case with spin S=1/2 is the natural one. Thus we discuss $H_{N,Z}$ on \mathcal{H}_N^f first and discuss the case of bosons later. The bottom of the spectrum of $H_{N,Z}$ is called ground-state energy

$$E_{NZ} := \inf \sigma(H_{NZ}). \tag{2.4}$$

At first, $E_{N,Z}$ does not need to be an eigenvalue of $H_{N,Z}$. The HVZ theorem, proved by Zhislin [Zhi6o], van Winter [vW64] and Hunziker [Hun66] shows that the essential spectrum of $H_{N,Z}$ is given by $\sigma_{\rm ess}$ ($H_{N,Z}$) = [$E_{N-1,Z}$, ∞). Thus the *binding condition*

$$E_{N,Z} < E_{N-1,Z} \tag{2.5}$$

ensures that there is some discrete spectrum below the essential spectrum, hence the atom can bind N electrons. In particular, (2.5) ensures that $E_{N,Z}$ is an eigenvalue of $H_{N,Z}$, i.e., there exists a function $\psi_{N,Z}$ such that

$$H_{N,Z}\psi_{N,Z} = E_{N,Z}\psi_{N,Z}. \tag{2.6}$$

Thus it is natural to call

$$N_c(Z) := \max\{N \in \mathbb{N} : E_{N,Z} < E_{N-1,Z}\}$$

the critical number of particles that an atom of charge Z can bind.

In this paper, we derive new bounds on $N_c(Z)$. The strategy of our proof is inspired by [Lie76] and, in particular, [Nam12]. One assumes (2.6) with $E_{N,Z} < E_{N-1,Z}$ for fixed nuclear charge Z > 0 (not necessarily an integer) which will then lead to a contradiction if N is too large. We sketch the original Bunguria–Lieb argument together with Nam's improvement in Section 3.

Our main result is

Theorem 2.2. Let $s \in (1,3]$ then there exists c(s) > 0 such that

$$N_c(Z) < b(s) Z + c(s) Z^{1/3}$$

where

$$b(s) := \max_{0 \le t \le 1} \frac{1 + t^{s-1}}{1 + t^s}.$$
 (2.7)

Remark 2.3. We conjecture that Theorem 2.2 holds for any $s \ge 1$ with the same b(s) and some $c(s) < \infty$ with $c(s) \to \infty$ as $s \to \infty$.

We prove Theorem 2.2 in Section 7. Finding good bounds on c(s) is technical, we study the cases s = 2 and s = 3 in greater detail. In particular, for s = 2 we show

Proposition 2.4. For any $Z \geq 2$

$$N_c(Z) < \frac{1}{2}(\sqrt{2}+1)Z + 2.96Z^{1/3}$$
 (2.8)

where $1.2071 < \frac{1}{2}(\sqrt{2} + 1) < 1.2072$.

For s = 3 we show

Proposition 2.5. For any $Z \geq 4$

$$N < b(3)Z + 3.90Z^{1/3} + 0.0134 + 0.184Z^{-1/3} + 0.0196Z^{-2/3},$$
(2.9)

with

1.1184 <
$$b(3) = \frac{2}{3} \frac{\sqrt[3]{1 + \sqrt{2}}}{(1 + \sqrt{2})^{2/3} - 1} < 1.1185$$
.

Remark 2.6. Proposition 2.4 improves the bound $N_c(Z) < 2Z + 1$ in [Lie84] for Z > 5.3. Since the constant $(\sqrt{2}+1)/2$ is slightly better than the one in [Nam12] it improves the result of [Nam12] for all $Z \ge 2$. For $Z \ge 35.8$ the bound in (2.9) is better than (2.8). In particular Proposition 2.4 shows

$$N < 1.12Z + 4Z^{1/3}, \quad Z \ge 4$$
.

We prove Propositions 2.4 and 2.5 in Section 7.

Proposition 2.5 significantly improves upon the results of [Nam12] for large Z. More importantly, while it falls short of proving the asymptotic neutrality of fermionic atoms, it provides the first quantitative result showing that, for atoms, the distinction between fermions and bosons is crucial. In [BL83] Benguria and Lieb showed that in contrary to fermions for bosonic atoms

$$\lim_{Z\to\infty}\frac{N_c(Z)}{Z}=t_c>1.$$

In fact, Benguria and Lieb proved the lower bound $\liminf_{Z\to\infty}\frac{N_c(Z)}{Z}\geq t_c$. Solovej showed the complementary bound $\limsup_{Z\to\infty}\frac{N_c(Z)}{Z}=t_c$ in [Sol90]. Numerically one finds $t_c\approx 1.21$ (see [Bau84]). Thus large bosonic atoms can have an ex-

Numerically one finds $t_c \approx 1.21$ (see [Bau84]). Thus large bosonic atoms can have an excess charge of 21 %. On the other hand, as proven in [LSST88], fermionic atoms are asymptotically neutral. Our bound (2.9) shows that fermionic atoms are very much different from bosonic atoms not only in the limit of infinite nuclear charge Z, but also, quantitatively, for large but finite nuclear charge. The constant $\frac{1}{2}(\sqrt{2}+1) < 1.2072$ in our bound (2.8) is just a bit smaller than $t_c \approx 1.21$, so it does not allow for this conclusion if one also allows for possible numerical uncertainties in the calculation of the precise value of t_c . However, the constant b(3) < 1.1185 in the leading order term of (2.9) is certainly much smaller than t_c , including possible numerical errors in the calculation of t_c .

Thus our results, in particular Proposition 2.5, show that fermionic atoms are quantitatively quite different from bosonic atoms, not only in the limit of large nuclear charges but already for medium values of Z. We apply our method to bosonic atoms in a forthcoming paper.

3. THE BENGURIA-LIEB-NAM ARGUMENT: PLAYING WITH WEIGHTS

Based on an idea by Benguria, Lieb showed $N_c < 2Z + 1$ for any $Z \ge 1$ in [Lie84]. One starts by taking the scalar product of the solution of the Schrödinger equation

$$H_{N,Z}\psi_{N,Z} = E_{N,Z}\psi_{N,Z} \tag{3.1}$$

with $|x_k| \psi_{N,Z}$ where x_k is the position of the k^{th} electron. Using an idea of Benguria allows to control the terms involving the electron–electron repulsion which together with a crucial positivity of the weighted kinetic energy term $\text{Re}\langle |x_k|\psi,P^2\psi\rangle$ leads to the bound N<2Z+1 under the binding condition (2.5). This led to the first non–asymptotic quantitative bound for the number of particles an atom can bind for arbitrary Z>0 We sketch more of the main ideas shortly.

In [Nam12] Nam used a similar approach but changed the weight from $|x_k|$ to $|x_k|^2$. This change in weight complicated the analysis considerably. Mainly because $\text{Re}\langle |x_k|\psi,P^2\psi\rangle$ is no longer positive anymore but also because with Nam's choice of weight the analysis of the terms including the electron–electron repulsion gets considerably more involved. Nevertheless, Nam was able to prove $N_c(Z) < 1.22Z + 3Z^{1/3}$ with the help of his new choice of weight, a breakthrough compared to the bound of Benguria–Lieb.

We refer to [Nam22] for a recent and comprehensive review, which includes a discussion of what we would call the *Benguria-Lieb-Nam Argument*. In this work, we follow a similar strategy but modify the power in the ansatz to a general power $|x|^s$ with $s \in (1,3]$. The case s = 1 is the case treated by Lieb in [Lie84]. The idea is the following. Assume we have a solution $\psi_{N,Z}$ of (3.1). Let $k \in \{1, 2, ..., N\}$ and multiply the Schrödinger equation from the left by $|x_k|^s \overline{\psi_{N,Z}}$, then, in the quadratic form sense,

$$0 = \langle |x_k|^s \psi_{N,Z}, (H_{N,Z} - E_{N,Z})\psi_{N,Z} \rangle = \text{Re}\langle |x_k|^s \psi_{N,Z}, (H_{N,Z} - E_{N,Z})\psi_{N,Z} \rangle.$$
(3.2)

Note that $\psi_{N,Z}$ is a many–particle function and the inner product above is the scalar product in the many–particle Hilbert space \mathcal{H}_N given in (2.2). For an introductory explanation, see,

for example, [LSo₉, Chapter ₃]. We ignore the spin, for now, since it is irrelevant to the argument. It is only relevant for bounds of the kinetic energy.

We want to single out the k^{th} particle. Let $N(k) := \{1, 2, 3, ... N\} \setminus \{k\}$. Then the atomic operator $H_{N,Z}$ for N particles, defined (2.1), can be written as

$$H_{N,Z} = \frac{1}{2}P_k^2 - \frac{Z}{|x_k|} + \sum_{i \in N(k)} \frac{1}{|x_i - x_k|} + H_{N-1,Z}^{(k)}.$$
 (3.3)

with

$$H_{N-1,Z}^{(k)} = \sum_{\substack{i=1\\i\neq k}}^{N} \left(\frac{1}{2}P_i^2 - \frac{Z}{|x_i|}\right) + \sum_{\substack{i,j \in N(k)\\i < i}} \frac{1}{|x_i - x_j|}.$$

the operator of an N-1 particle system where the k^{th} particle is removed. Combining (3.2) and (3.3) we find

$$0 = \operatorname{Re}\left(|x_{k}|^{s} \psi_{N,Z}, \left[\frac{1}{2} P_{k}^{2} - \frac{Z}{|x_{k}|} + \sum_{i \in N(k)} \frac{1}{|x_{i} - x_{k}|}\right] \psi_{N,Z}\right) + \operatorname{Re}\langle|x_{k}|^{s} \psi_{N,Z}, (H_{N-1,Z}^{(k)} - E_{N,Z})\psi_{N,Z}\rangle.$$

$$(3.4)$$

From (2.5) we have $H_{N-1,Z}^{(k)} \ge E_{N-1}$. Since $H_{N-1,Z}^{(k)}$ commutes with $|x_k|^s$ and for fixed x_k the function $|x_k|^s \psi$ has the same symmetry as ψ in the other N-1 variables, we have

$$\operatorname{Re}\langle |x_{k}|^{s} \psi_{N,Z}, (H_{N-1,Z}^{(k)} - E_{N,Z}) \psi_{N,Z} \rangle$$

$$= \langle |x_{k}|^{s/2} \psi_{N,Z}, (H_{N-1,Z}^{(k)} - E_{N,Z}) |x_{k}|^{s/2} \psi_{N,Z} \rangle \ge 0.$$
(3.5)

Combining (3.4) and (3.5) we arrive at

$$0 \ge \frac{1}{2} \operatorname{Re} \left\langle |x_k|^s \psi_{N,Z}, P_k^2 \psi_{N,Z} \right\rangle - Z \left\langle \psi_{N,Z}, |x_k|^{s-1} \psi_{N,Z} \right\rangle + \sum_{i \in N(k)} \left\langle \psi_{N,Z}, \frac{|x_k|^s}{|x_i - x_k|} \psi_{N,Z} \right\rangle.$$

$$(3.6)$$

Of course, $\langle |x_k|^s \psi_{N,Z}, P_k^2 \psi_{N,Z} \rangle = \langle \nabla_k (|x_k|^s \psi_{N,Z}), \nabla_k \psi_{N,Z} \rangle$ in the quadratic form sense, where ∇_k is the gradient with respect to the position of the k^{th} particle.

Due to the symmetry of the ground state, see (2.3), the first two terms of (3.6) do not depend on k. Consequently by summing over $k \in \{1, 2, ..., N\}$ we arrive at

$$0 \ge \frac{1}{2} \operatorname{Re} \left\langle \nabla_{1}(|x_{1}|^{s} \psi_{N,Z}), \nabla_{1} \psi_{N,Z} \right\rangle - Z \left\langle |x_{1}|^{s-1} \psi_{N,Z}, \psi_{N,Z} \right\rangle + \frac{1}{N} \sum_{k=1}^{N} \sum_{j \in N(k)} \left\langle \psi_{N,Z}, \frac{|x_{k}|^{s}}{|x_{j} - x_{k}|} \psi_{N,Z} \right\rangle.$$
(3.7)

Symmetrizing the double sum above yields

$$\frac{1}{N} \sum_{k=1}^{N} \sum_{i \in N(k)} \left\langle \psi_{N,Z}, \frac{|x_{k}|^{s}}{|x_{i} - x_{k}|} \psi_{N,Z} \right\rangle = \frac{1}{2N} \sum_{k=1}^{N} \sum_{j \in N(k)} \left\langle \psi_{N,Z}, \frac{|x_{j}|^{s} + |x_{k}|^{s}}{|x_{j} - x_{k}|} \psi_{N,Z} \right\rangle
= \frac{1}{N} \sum_{\substack{j,k=1 \ j < k}}^{N} \left\langle \psi_{N,Z}, \frac{|x_{j}|^{s} + |x_{k}|^{s}}{|x_{j} - x_{k}|} \psi_{N,Z} \right\rangle.$$
(3.8)

For $N \in \mathbb{N}$ with $N \ge 2$ we define

$$\alpha_{N,s} := \inf \left\{ \frac{\sum_{1 \le j < k \le N} \frac{|x_j|^s + |x_k|^s}{|x_j - x_k|}}{(N-1) \sum_{k=1}^N |x_k|^{s-1}} : x_k \in \mathbb{R}^3 \text{ for } k = 1, \dots, N \right\}$$
(3.9)

which for s = 2 was introduced by Nam in [Nam12, Equation (1)]. Combining (3.7) and (3.8) and using the definition of $\alpha_{N,s}$ yields

$$\alpha_{N,s}(N-1) < Z - \frac{1}{2} \frac{\text{Re}\left\langle \nabla_1(|x_1|^s \psi_{N,Z}), \nabla_1 \psi_{N,Z} \right\rangle}{\left\langle |x_1|^{s-1} \psi_{N,Z}, \psi_{N,Z} \right\rangle}.$$
(3.10)

Remark 3.1. The bound (3.10) is the starting point for our analysis. The problem is now reduced to find good lower bounds for $\alpha_{N,s}$ and the second term in the right–hand side of (3.10). Numerical approximation of the values of $\alpha_{N,s}$ for various are given in Figure 1.

When s=1 we have $\alpha_{N,s}\geq 1/2$ since $|x|+|y|\geq |x-y|$ by the triangle inequality. Also Re $\langle \nabla_1(|x_1|\varphi), \nabla_1\varphi\rangle = \left\langle \nabla_1(|x_1|^{1/2}\varphi), \nabla_1(|x_1|^{1/2}\varphi)\right\rangle - \frac{1}{4}\left\langle \varphi, |x_1|^{-1}\varphi\right\rangle > 0$, using the IMS localization formula and Hardy's inequality in dimension three. Thus the second term on the right-hand-side of (3.10) can be dropped when s=1 and one recovers Lieb's result in the case of a single atom directly.

It is not too hard to see that for all $s \ge 1$ one has $\alpha_{2,s} = 1/2$ as well. Besides these two cases, s = 1 and general $N \in \mathbb{N}$, respectively, N = 2 and general $s \ge 1$, it is nontrivial to find good lower bounds for $\alpha_{N,s}$. Such a bound was derived for $\alpha_{N,2}$ in [Nam12]. For Nam's argument it was essential to have s = 2. He also showed that $\alpha_{N,2}$ is monotone increasing in N. This holds for general $s \ge 1$.

Lemma 3.2. $\alpha_{N,s}$ is increasing in $N \in \mathbb{N}$ for all $s \geq 1$.

Proof. In fact, Nam's original proof carries over with minor changes in notation. For the convenience of the reader, we give the short argument. Singling out the particle *m*, we have

$$\sum_{1 \le j < k \le N} \frac{\left| x_j \right|^s + |x_k|^s}{|x_j - x_k|} = \sum_{m=1}^N \left(\frac{1}{N-2} \sum_{\substack{1 \le j < k \le N \\ j \ne m, k \ne m}} \frac{\left| x_j \right|^s + |x_k|^s}{|x_j - x_k|} \right)$$

$$\geq \sum_{m=1}^N \left(\alpha_{N-1,s} \sum_{\substack{k=1 \\ k \ne m}}^N |x_k|^s \right) = \alpha_{N-1,s} (N-1) \sum_{k=1}^N |x_k|^s$$

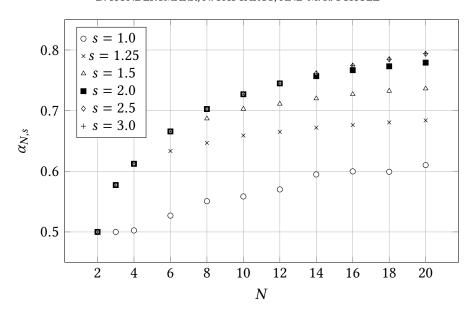


FIGURE 1. Numerical approximation of the values of $\alpha_{N,s}$ for various s and N. Starting from an initial sample set of vectors the values of $\alpha_{N,s}$ have been obtained using a Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm implemented in Python. For s=2.5 and s=3.0 the values of $\alpha_{N,s}$ seem to be almost identical for $N\leq 20$. In the plot $\alpha_{16,1}>\alpha_{18,1}$ which is contrary to Lemma 3.2 and due to the fat that numerical approximation is difficult for small $s\geq 1$.

using the definition of $\alpha_{N-1,s}$. This shows that $\alpha_{N,s} \leq \alpha_{N+1,s}$ for all $N \in \mathbb{N}$.

Lemma 3.2 shows that $\alpha_{N,s}$ is increasing in N, so once it is bounded, it has a limit. Dividing the denominator and numerator in the definition of $\alpha_{N,s}$ by N^2 suggests the following meanfield type approximation

$$\beta_{s} := \inf \left\{ \frac{\iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\mu(x) d\mu(y)}{\int_{\mathbb{R}^{3}} |x|^{s - 1} d\mu(x)} : \mu \in P\left(\mathbb{R}^{3}\right) \right\}, \tag{3.11}$$

where $P(\mathbb{R}^3)$ is the set of probability measures on \mathbb{R}^3 . In fact, for technical reasons, we will additionally assume further regularity of the probability measures μ in the definition of β_s , see (4.1) below.

Lemma 3.3. For all $N \in \mathbb{N}$ and $s \ge 1$ we have $\alpha_{N,s} \le \beta_s$.

Proof. Again, the proof follows the argument in [Nam12]. By symmetry,

$$\iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\mu(x) d\mu(y) = \frac{1}{N} \int_{\mathbb{R}^{3N}} \frac{1}{N - 1} \sum_{1 \le j < k \le N} \frac{|x_{j}|^{s} + |x_{k}|^{s}}{2|x_{j} - x_{k}|} d\mu(x_{1}) \dots d\mu(x_{N})$$

$$\ge \frac{\alpha_{N,s}}{N} \int_{\mathbb{R}^{3N}} \sum_{k=1}^{N} |x_{k}|^{s-1} d\mu(x_{1}) \dots d\mu(x_{N}) = \alpha_{N,s} \int_{\mathbb{R}^{3}} |x|^{s-1} d\mu(x) .$$

Thus $\alpha_{N,s} \leq \beta_s$ for all $N \in \mathbb{N}$ and $s \geq 1$.

Remark 3.4. Given the monotonicity of $\alpha_{N,s}$ in N and the fact that mean-field expressions such as (3.11) often are an excellent approximation for many particle expression such as the one for $\alpha_{N,s}$, one expects that $\alpha_{N,s}$ converges to β_s in the limit of large N. This is indeed the case, Lemma 5.5 shows that $\lim_{N\to\infty}\alpha_{N,s}=\beta_s$ for all $s\geq 2$, see Remark 5.6.

That leaves us with the task of finding the value of β_s , or, at least, good lower bounds for it. Nam conjectured in [Nam12] that the infimum in the definition of β_2 is achieved by radially symmetric probability measures μ . If this is the case, then one can easily find *excellent lower bounds* for β_2 , and also β_s . In the next section, we show that indeed the infimum is achieved with radial measures, not only for s=2 but even in the range $0 \le s \le 3$. This allows us to tighten the lower bound for β_2 and it also yields excellent lower bounds for β_s in the range $0 \le s \le 3$.

In Section 5 we then show how to derive lower bounds for $\alpha_{N,s}$ in terms of β_s . This works for all $s \geq 2$, but using the lower bounds for β_s derived in Section 4 requires to restrict our studies to $2 \leq s \leq 3$. In the limit $s \to 1$ our estimate reduces to the estimate found by Lieb and in the case s = 2 we find a new improved estimate sharpening the results in [Nam12]. We can further improve the results by choosing $s \in (1,3]$ optimally.

In Section 6, we derive upper bounds for the right-hand side of (3.10). In Section 7, we prove the main Theorem 2.2 along with Propositions 2.4 and 2.5.

4. Symmetry of minimizing sequences

First, we give a more careful definition of β_s . From now on we set, for $s \ge 1$,

$$\beta_{s} := \inf \left\{ \frac{\iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\mu(x) d\mu(y)}{\int_{\mathbb{R}^{3}} |x|^{s - 1} d\mu(x)} : \mu \in D_{s}(\mathbb{R}^{3}) \right\}. \tag{4.1}$$

where $D_s(\mathbb{R}^3) = P(\mathbb{R}^3) \cap H^{-1}(\mathbb{R}^3) \cap L_{s-1}(\mathbb{R}^3)$. Here $P(\mathbb{R}^3)$ is the set of all probability measures in \mathbb{R}^3 , H^{-1} is the usual Sobolev space of negative order

$$H^{-1}(\mathbb{R}^d) = \left\{ f \in \mathcal{S}^*(\mathbb{R}^d) : \|f\|_{H^{-1}} = \left(\int_{\mathbb{R}^d} \frac{|\widehat{f}(k)|^2}{1 + |k|^2} \, dk \right)^{1/2} < \infty \right\}$$

where $S^*(\mathbb{R}^d)$ is the space of tempered distributions, \widehat{f} the Fourier transform of a tempered distribution f, and $L_t(\mathbb{R}^3)$ the set of all finite signed or complex–valued measures for which $\int_{\mathbb{R}^3} |x|^t d|\mu|(x) < \infty$, where $|\mu|$ is the total variation of μ . First, we show that for $1 \le s \le 3$ the infimum in (4.1) can be computed using only radially

First, we show that for $1 \le s \le 3$ the infimum in (4.1) can be computed using only radially symmetric probability measures.

Definition 4.1. Let $\rho \in P(\mathbb{R}^3)$. The radial part of ρ is the measure $\overline{\rho}$ given by

$$\int_{\mathbb{R}^3} f(x) d\overline{\rho}(x) := \int_{\mathbb{R}^3} \int_{SO(3)} f(U^{-1}x) \ dU d\rho(x), \tag{4.2}$$

for any bounded measurable function f where dU is the normalized Haar measure on SO(3). We say that a probability measure ρ is radial if $\rho = \overline{\rho}$. The set of radial probability measures

on \mathbb{R}^3 is given by

$$P_{\mathrm{rad}}(\mathbb{R}^3) := \left\{ \rho \in P(\mathbb{R}^3) : \rho = \overline{\rho} \right\} .$$

With this definition, we have

Theorem 4.2. For all $1 \le s \le 3$ we have

$$\beta_{s} = \beta_{s}^{rad} := \inf \left\{ \frac{\iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\mu(x) d\mu(y)}{\int_{\mathbb{R}^{3}} |x|^{s - 1} d\mu(x)} : \mu \in D_{s, rad}(\mathbb{R}^{3}) \right\}.$$
(4.3)

where $D_{s,rad}(\mathbb{R}^3) = P_{rad}(\mathbb{R}^3) \cap H^{-1}(\mathbb{R}^3) \cap L_{s-1}(\mathbb{R}^3)$.

The proof of this theorem is based on

Lemma 4.3. Let $\rho \in P(\mathbb{R}^3) \cap H^{-1}(\mathbb{R}^3)$ and

$$I_s(\rho) := \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x - y|} d\rho(x) d\rho(y) . \tag{4.4}$$

Then for any $s \in (1,3]$

$$I_s(\rho) \geq I_s(\overline{\rho})$$

where $\overline{\rho}$ is the radial part of ρ .

Remark 4.4. I_0 is the Coulomb energy, which is known to be positive definite, that is, $I_0(\rho) \ge 0$ for all signed and even complex–valued measures (see [Göo3], or [LSo9, Theorem 5.1]). From positive definiteness the bound $I_0(\rho) \ge I_0(\overline{\rho})$ follows easily. Indeed let $\nu = \rho - \overline{\rho}$ be the non–radial part of ρ and also define the bilinear version $I_0(\rho_1, \rho_2) = \iint \frac{1}{|x-y|} d\rho_1(x) d\rho_2(y)$. Then

$$I_0(\rho) = I_0(\overline{\rho} + \nu, \overline{\rho} + \nu) = I_0(\overline{\rho}, \overline{\rho}) + 2I_0(\overline{\rho}, \nu) + I_0(\nu, \nu)$$

Since $\overline{\rho}$ is a radial measure, Newtons theorem shows that its potential, given by $V_{\overline{\rho}}(y) = \int \frac{1}{|x-y|} d\overline{\rho}(x) = \int \frac{1}{\max(|x|,|y|)} d\overline{\rho}(x) = V_{\overline{\rho}}(|y|)$ is also radial, hence

$$I_0(\overline{\rho}, \nu) = \frac{1}{2} \int V_{\overline{\rho}}(|y|) d\nu(y) = 0$$

since the non-radial part ν is orthogonal to radial functions. Hence

$$I_0(\rho) = I_0(\overline{\rho}) + I_0(\nu) \ge I_0(\overline{\rho})$$
.

Unfortunately, we don't know of any such simple argument based on positive definiteness, or variations thereof, for I_s when s > 0.

Since the proof of Lemma 4.3 is a bit lengthy, we postpone it to the end of this section and will first show how it implies Theorem 4.2 and discuss its consequences. We will always assume $s \ge 1$ in the following.

Proof of Theorem 4.2. In the definition of β_s , the infimum is taken over quotients of the form $I_s(\rho)/(\int |x|^{s-1}d\rho(x))$. The denominator does not change under radial symmetrization, i.e., we have

$$\int |x|^{s-1} d\rho(x) = \int |x|^{s-1} d\overline{\rho}(x)$$

where $\overline{\rho}$ is the radial part of ρ . Note that $\overline{\rho}$ is again a probability measure and it is also in H^{-1} . By Lemma 4.3 we have $I_s(\rho) \ge I_s(\overline{\rho})$ when $1 \le s \le 3$. So for this range of parameters s we have

$$\frac{I_s(\rho)}{\int |x|^{s-1}d\rho(x)} \ge \frac{I_s(\overline{\rho})}{\int |x|^{s-1}d\overline{\rho}(x)},$$

which implies (4.3).

Equipped with Theorem 4.2 we can compute a lower bound to β_s when $1 < s \le 3$.

Proposition 4.5. Let $s \in (1,3]$ and let β_s be defined as in (4.1) then

$$\beta_s \ge \min_{t \in [0,1]} \frac{1+t^s}{1+t^{s-1}} = \frac{s}{s-1} t_0 =: b(s)^{-1}$$

where $t_0 \in (0, 1)$ is the unique root of $t \mapsto t^s + st + 1 - s$ in (0, 1).

Proof. By definition and Lemma 4.3 we have for any $s \in [1, 3]$

$$\beta_{s} \geq \inf \left\{ \frac{\iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} (d\overline{\rho}(x) d\overline{\rho}(y)}{\int_{\mathbb{R}^{3}} |x|^{s - 1} d\overline{\rho}(x)} : \overline{\rho} \in P_{\text{rad}}(\mathbb{R}^{3}) \cap H^{-1}(\mathbb{R}^{3}) \right\}$$

where the infimum is taken only over radial probability measures $\overline{\rho}$. Using Newtons Theorem [LSo9, Theorem 5.2] for fixed $\overline{\rho}$ yields

$$\iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x - y|} d\overline{\rho}(x) d\overline{\rho}(y) = \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|x|^s + |y|^s}{\max(|x|, |y|)} d\overline{\rho}(x) d\overline{\rho}(y).$$

Therefore, with $t(x, y) = \frac{\min(|x|, |y|)}{\max(|x|, |y|)} = \min\left(\frac{|x|}{|y|}, \frac{|y|}{|x|}\right)$,

$$\frac{1}{2} \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{|x - y|} d\overline{\rho}(x) d\overline{\rho}(y)
= \frac{1}{2} \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{\max(|x|, |y|)(|x|^{s-1} + |y|^{s-1})} (|x|^{s-1} + |y|^{s-1}) d\overline{\rho}(x) d\overline{\rho}(y)
= \frac{1}{2} \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{1 + t(x, y)^{s}}{1 + t(x, y)^{s-1}} (|x|^{s-1} + |y|^{s-1}) d\overline{\rho}(x) d\overline{\rho}(y)
\geq \min_{0 \le t \le 1} \frac{1 + t^{s}}{1 + t^{s-1}} \int_{\mathbb{R}^{3}} |x|^{s-1} d\overline{\rho}(x) .$$

Consequently,

$$\beta_s \ge \min_{t \in [0,1]} \frac{1+t^s}{1+t^{s-1}}.$$
 (4.5)

While this minimum can easily be computed for s = 2 and s = 3, it cannot be computed in a closed form for arbitrary 2 < s < 3. The minimum is obviously not attained at the boundary $t \in \{0, 1\}$ since

$$\frac{1+\left(\frac{1}{2}\right)^s}{1+\left(\frac{1}{2}\right)^{s-1}} = \frac{2^s+1}{2^s+2} < 1.$$

We locate the position of the minimum by differentiating

$$\left(\frac{1+t^s}{1+t^{s-1}}\right)' = \frac{t^s(t^s+s(t-1)+1)}{(t^s+t)^2}$$

which vanishes for $t_0 \in (0, 1)$ iff

$$t_0^s + st_0 + 1 - s = 0. (4.6)$$

The minimum in equation (4.5) is therefore attained at $t_0 \in (0, 1)$. Combining the equation (4.6) and (4.5) shows

$$\beta_s \ge \min_{t \in [0,1]} \frac{1+t^s}{1+t^{s-1}} = \frac{s}{s-1} t_0 = b(s)^{-1}.$$

Remark 4.6. Nam conjectured in [Nam12] that β_2 could be calculated using only radial probability measures. Theorem 4.2 shows that this is indeed correct. Because of this, our lower bound for β_2 is slightly better than the one in [Nam12]. More importantly, the main improvement in our analysis of the ionization problem comes from the fact that the lower bound for β_s is increasing in $s \in [2, 3]$ and substantially bigger than β_2 when s is close to 3. We would like to take s much larger than 2, however, we do not know whether the lower bound of Proposition 4.5 extends to s > 3.

For s = 2 and s = 3, one can compute the value of β_s explicitly. One finds

$$\beta_2 = 2(\sqrt{2} - 1) \Rightarrow b(2) = \frac{1}{2}(\sqrt{2} + 1) \le 1.2072$$

$$\beta_3 = \frac{3}{2} \frac{(1 + \sqrt{2})^{2/3} - 1}{\sqrt[3]{1 + \sqrt{2}}} \Rightarrow b(3) = \frac{2}{3} \frac{\sqrt[3]{1 + \sqrt{2}}}{(1 + \sqrt{2})^{2/3} - 1} \le 1.1185$$

To find upper bounds on β_s , respectively lower bounds on b(s), one can choose an explicit measure in (4.3). To produce Figure 2 we have chosen

$$\overline{\rho}_{num}(x) = \begin{cases} A |x|^{-p}, & |x| \in [1, n] \\ 0, & |x| \notin [1, n] \end{cases}.$$

and have optimized numerically in the parameters p and n and chose A>0 such that $\overline{\rho}_{num}$ is the density of a probability measure. The results of this study are plotted in Figure 2 where $b_{num}(s)$ are the numerically obtained lower bounds on β_s^{-1} after the optimization explained above.

Next, we give the

Proof of Lemma 4.3. Before we give a detailed proof let us clarify the strategy. We would like to mimic the strategy for the Coulomb potential I_0 outlined in Remark 4.4, but the weight $|x|^s$ seems to spoil the argument and, as far we know, no arguments using positive definiteness, as for I_0 , or conditional positive definiteness, i.e, $I_s(v) \ge 0$ for all (suitable) signed measures v with toal mass $v(\mathbb{R}^3) = 0$, seem to be available. So we have to use a different route. Introduce again the bilinear version

$$I_{s}(\rho_{1}, \rho_{2}) = \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\rho_{1}(x) d\rho_{2}(y).$$
(4.7)

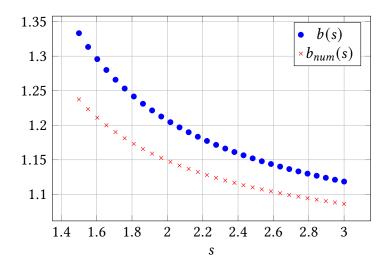


FIGURE 2. Values of b(s) according to Proposition 4.5, where t_0 was computed numerically. The lower bounds $b_{num}(s)$ on β_s^{-1} have been found by choosing explicit measures in (4.3) and numerical optimization. The exact value of β_s^{-1} has to be between both lines. The values b(3) and $b_{num}(3)$ differ by approximately 3%.

Then as for I_0 we have

$$I_s(\rho) = I_s(\overline{\rho}) + 2I_s(\overline{\rho}, \nu) + I_s(\nu)$$

where $v = \rho - \overline{\rho}$ is the non-radial part of ρ . Since $\overline{\rho}$ is a radial measure, Newton's theorem shows again that the functions

$$\int \frac{|x|^s}{|x-y|} d\overline{\rho}(x) = \int \frac{|x|^s}{\max(|x|,|y|)} d\overline{\rho}(x) =: V_1(|y|),$$

$$\int \frac{1}{|x-y|} d\overline{\rho}(x) = \int \frac{1}{\max(|x|,|y|)} d\overline{\rho}(x) =: V_2(|y|)$$

are radial. Thus

$$2I_s(\overline{\rho}, \nu) = \int_{\mathbb{R}^3} V_1(|y|) d\nu(y) + \int_{\mathbb{R}^3} V_2(|y|) |y|^s d\nu(y) = 0$$
 (4.8)

since the measure ν is orthogonal to radial functions. Thus it is enough to show that $I_s(\nu) \ge 0$ for measures ν which are orthogonal to radial functions. Note that the potential $V_{\mu} = \int \frac{1}{|x-y|} d\mu(y)$ solves the equation

$$-\Delta V_{\mu} = 4\pi\mu$$

in the sense of distributions. Hence, at least informally,

$$I_{s}(\mu) = \int_{\mathbb{R}^{3}} |x|^{s} \int_{\mathbb{R}^{3}} \frac{1}{|x-y|} d\mu(x) d\mu(y) = \int_{\mathbb{R}^{3}} |x|^{s} V_{\mu}(x) d\mu(x)$$
$$= \frac{1}{4\pi} \int |x|^{s} V_{\mu}(x) (-\Delta V_{\mu}(x)) dx = \frac{1}{4\pi} \left\langle |x|^{s} V_{\mu}, -\Delta V_{\mu} \right\rangle$$

where $\langle \cdot, \cdot \rangle$ is the usual scalar product on $L^2(\mathbb{R}^3)$ and we used symmetry for the first equality. Since μ is real-valued, so is its potential V_{μ} , hence using the IMS formula and Hardy's inequality, there exists a $c_H > 0$ such that

$$4\pi I_{s}(\mu) = \operatorname{Re}\langle |x|^{s} V_{\mu}, -\Delta V_{\mu} \rangle = \langle |x|^{s/2} V_{\mu}, -\Delta (|x|^{s/2} V_{\mu}) \rangle - \langle V_{\mu}, \frac{s^{2}}{4} |x|^{s-2} V_{\mu} \rangle$$
$$= \left\langle |x|^{s/2} V_{\mu}, \left[-\Delta - \frac{s^{2}}{4|x|^{2}} \right] (|x|^{s/2} V_{\mu}) \right\rangle \ge \left(c_{H} - \frac{s^{2}}{4} \right) \langle V_{\mu}, |\cdot|^{s-2} V_{\mu} \rangle$$

Using $\mu = \nu = \rho - \overline{\rho}$ above and noting that ν is orthogonal to radial functions one sees that also its potential V_{ν} is orthogonal to radial functions. Hence

$$4\pi I_s(\nu) \ge \left(c_H - \frac{s^2}{4}\right) \langle V_{\nu}, |\cdot|^{s-2} V_{\nu} \rangle$$

with the improved Hardy constant $c_H = d^2/4$ in dimension $d \ge 2$, (see [EFo6, Lemma 2.4]), since the potential V is orthogonal to radial symmetric functions in the L^2 -sense. Hence $I_s(\nu) = I_s(\rho - \overline{\rho}) \ge 0$ whenever $s \le d = 3$. Of course, this is not a proof, the weight $|x|^s$ is not bounded, so the application of the IMS localization formula is informal. In addition, it is not clear that the potential V_{ν} is well-defined.

To make this argument rigorous, one has to be a bit more careful. For any $x \in \mathbb{R}^3$, $\varepsilon, \lambda > 0$ and $\mu \in H^{-1}(\mathbb{R}^3)$ we define

$$\varphi_{\varepsilon,s}(x) := \frac{|x|^s}{1 + \varepsilon |x|^s}, \quad V_{\mu,\lambda}(x) := \int_{\mathbb{R}^3} \frac{e^{-\lambda|x-y|}}{4\pi |x-y|} d\mu(y), \tag{4.9}$$

These are regularized versions of the weight $|x|^s$ and the potential V_{ν} , respectively. Let us collect some properties of $\varphi_{\varepsilon,s}$, $V_{\lambda,\mu}$ and $u[\mu]$ before we continue. Note that $V_{\mu,\lambda}$ is the solution to the differential equation

$$(-\Delta + \lambda^2)V_{\mu,\lambda} = \mu. \tag{4.10}$$

in the sense of distributions. It is elementary to verify that $\varphi_{\varepsilon,s} \in W^{1,\infty}$ since $x \mapsto |x|^s$ is weakly differentiable and $\varphi_{\varepsilon,s}$ is bounded by construction. In the definition of β_s in (4.1) we also assumed that $\mu \in H^{-1}(\mathbb{R}^d)$. This ensures that $V_{\mu,\lambda} \in H^1$. Indeed, (4.10) shows that the Fourier transform of $V_{\lambda,\nu}$ is given by $\widehat{V}_{\lambda,\mu}(k) = (|k|^2 + \lambda)^{-1}\widehat{\mu}(k)$. Hence the H^{-1} norm of $V_{\lambda,\nu}$ is given by

$$\int_{\mathbb{R}^{3}} (1+|k|^{2}) \left| \widehat{V}_{\mu,\lambda}(k) \right|^{2} dk \lesssim \int_{\mathbb{R}^{2}} \frac{(1+|k|^{2})}{\lambda^{2}+|k|^{2}} \frac{|\widehat{\mu}(k)|^{2}}{\lambda^{2}+|k|^{2}} dk \lesssim \int_{\mathbb{R}^{3}} \frac{|\widehat{\mu}(k)|^{2}}{\lambda^{2}+|k|^{2}} dk < \infty$$

The last integral is finite for any $\lambda > 0$ since, by assumption, $\mu \in H^{-1}$. In particular, we also have $\varphi_{\varepsilon}V_{\mu,\lambda} \in H^1$ for any $\varepsilon,\lambda > 0$ as a product of an $W^{1,\infty}$ and an H^1 function. Note that if we split a probability measure $\rho \in H^{-1}(\mathbb{R}^3)$ as $\rho = \overline{\rho} + \nu$, with $\overline{\rho}$ the radial and ν the non–radial parts, the same holds for the potential $V_{\overline{\rho}}$ and V_{ν} . Thus all potentials we need

are in $H^1(\mathbb{R}^3)$. By monotone convergence

$$I_{s}(\rho) = \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\rho(x) d\rho(y) = \lim_{\lambda \to 0} \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{(|x|^{s} + |y|^{s})e^{-\lambda|x - y|}}{2|x - y|} d\rho(y) d\rho(x)$$

$$= \lim_{\lambda \to 0} \lim_{\varepsilon \to 0} \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{(\varphi_{\varepsilon,s}(x) + \varphi_{\varepsilon,s}(y))e^{-\lambda|x - y|}}{2|x - y|} d\rho(y) d\rho(x)$$

$$(4.11)$$

Define

$$I_s^{\lambda,\varepsilon}(\rho) = \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{(\varphi_{\varepsilon,s}(x) + \varphi_{\varepsilon,s}(y))e^{-\lambda|x-y|}}{|x-y|} d\rho(y) d\rho(x)$$

and its bilinear version

$$I_s^{\lambda,\varepsilon}(\rho_1,\rho_2) = \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{(\varphi_{\varepsilon,s}(x) + \varphi_{\varepsilon,s}(y))e^{-\lambda|x-y|}}{|x-y|} d\rho_1(y) d\rho_1(x) .$$

Split ρ into its radial part $\overline{\rho}$ and its non-radial part $v = \rho - \overline{\rho}$. Then as in (4.7) one sees

$$I_s^{\lambda,\varepsilon}(\rho) = I_s^{\lambda,\varepsilon}(\overline{\rho}) + 2I_s^{\lambda,\varepsilon}(\overline{\rho},\nu) + I_s^{\lambda,\varepsilon}(\nu) .$$

Again we have that the potentials

$$\widetilde{V}_1 = (-\Delta_{\lambda})^{-1} \overline{\rho}$$
 and $\widetilde{V}_2 = (-\Delta_{\lambda})^{-1} \varphi_{\epsilon,s} \overline{\rho}$

are rotationally symmetric. Thus as in (4.8) we have

$$8\pi I_s^{\lambda,\varepsilon}(\overline{\rho},v) = \int_{\mathbb{R}^3} \widetilde{V}_1(|y|) dv(y) + \int_{\mathbb{R}^3} \widetilde{V}_2(|y|) |y|^s dv(y) = 0$$

since ν is a bounded measure orthogonal to radial functions. Thus we have

$$I_s^{\lambda,\varepsilon}(\rho) = I_s^{\lambda,\varepsilon}(\overline{\rho}) + I_s^{\lambda,\varepsilon}(\nu) \tag{4.12}$$

and the claim follows once we show that $I_s^{\lambda,\varepsilon}(\nu) \geq 0$ for $\nu = \rho - \overline{\rho}$.

We claim that for any probability measure $\mu \in P(\mathbb{R}^3) \cap H^{-1}(\mathbb{R}^3)$

$$\frac{1}{4\pi}I_{s}^{\lambda,\varepsilon}(\mu,\mu) = \left\langle \nabla(\varphi_{\varepsilon,s}V_{\lambda,\mu}), \nabla(V_{\lambda,\mu}) \right\rangle + \lambda \left\langle \varphi_{\varepsilon,s}^{1/2}V_{\lambda,\mu}, \varphi_{\varepsilon,s}^{1/2}V_{\lambda,\mu} \right\rangle \tag{4.13}$$

where $V_{\lambda,\mu} = (-\Delta + \lambda)^{-1}\mu$ and $\varphi_{\varepsilon,s}V_{\lambda,\nu} \in H^1(\mathbb{R}^3)$. Assuming this representation allows to finish the proof since now we can apply the IMS localization formula. Since the right-hand side of (4.13) is real, we have

$$\frac{1}{4\pi} I_{s}^{\lambda,\varepsilon}(\mu,\mu) = \operatorname{Re}\left\langle \nabla(\varphi_{\varepsilon,s}V_{\mu}), \nabla(V_{\mu}) \right\rangle + \lambda \left\langle \varphi_{\varepsilon,s}^{1/2} V_{\lambda,\mu}, \varphi_{\varepsilon,s}^{1/2} V_{\lambda,\mu} \right\rangle
= \left\langle \nabla(\varphi_{\varepsilon,s}^{1/2} V_{\mu}), \nabla(\varphi_{\varepsilon,s}^{1/2} V_{\mu}) \right\rangle - \left\langle V_{\mu}, |\nabla \varphi_{\varepsilon,s}^{1/2}|^{2} V_{\mu} \right\rangle + \lambda \left\langle \varphi_{\varepsilon,s}^{1/2} V_{\lambda,\mu}, \varphi_{\varepsilon,s}^{1/2} V_{\lambda,\mu} \right\rangle$$
(4.14)

from the IMS localization formula. Computing the derivative shows

$$|\nabla \varphi_{\varepsilon,s}^{1/2}|^2 = \varphi_{\varepsilon,s} \left| \frac{\nabla \varphi_{\varepsilon,s}(x)}{2\varphi_{\varepsilon,s}(x)} \right|^2 = \varphi_{\varepsilon,s} \frac{s^2}{4|x|^2},$$

so, since $\lambda \geq 0$,

$$\frac{1}{4\pi}I_{s}^{\lambda,\varepsilon}(\mu,\mu) \geq \left\langle \nabla(\varphi_{\varepsilon,s}^{1/2}V_{\mu}), \nabla(\varphi_{\varepsilon,s}^{1/2}V_{\mu}) \right\rangle - \left\langle \varphi_{\varepsilon,s}^{1/2}V_{\mu}, \frac{s^{2}}{4|x|^{2}}\varphi_{\varepsilon,s}^{1/2}V_{\mu} \right\rangle$$

We use this for $\mu = \nu = \rho - \overline{\rho} \in H^{-1}(\mathbb{R}^d)$. Note that ν being orthogonal to radial functions implies that its potential $V_{\nu} = (\Delta + \lambda)^{-1}\nu$ is orthogonal to radial functions in $L^2(\mathbb{R}^3)$. Also, since both ρ and $\overline{\rho} \in H^{-1}(\mathbb{R}^3)$ we also have that $\nu \in H^{-1}(\mathbb{R}^3)$, so we can use the representation (4.13) for $\mu = \nu$.

Hence with the improved Hardy inequality $\widetilde{C}_d^H=d^2/4$ (see [EFo6, Lemma 2.4]), valid for functions orthogonal to radial functions, we get

$$\frac{1}{4\pi}I_s^{\lambda,\varepsilon}(\nu,\nu) \ge \left(\widetilde{C}_3^H - s^2/4\right) \left\langle \varphi_{\varepsilon,s}^{1/2} V_{\nu}, |x|^{-2} \varphi_{\varepsilon,s}^{1/2} V_{\nu} \right\rangle. \tag{4.15}$$

In our case d=3, so (4.15) shows that $I_s(\nu,\nu)\geq 0$ as long as $s\leq 3$. Together with (4.12) we get

$$I_{s}(\rho) = \lim_{\varepsilon \to 0} \lim_{\lambda \to 0} I_{s}^{\lambda,\varepsilon}(\rho) \ge \lim_{\varepsilon \to 0} \lim_{\lambda \to 0} I_{s}^{\lambda,\varepsilon}(\overline{\rho}) = I_{s}(\overline{\rho})$$
(4.16)

for any measure $\rho \in P(\mathbb{R}^3) \cap H^{-1}(\mathbb{R}^3)$ and all $0 \le s \le 3$.

It remains to prove the representation (4.13). First note that by symmetry we have

$$\frac{1}{4\pi}I_{S}^{\lambda\varepsilon}(\mu,\mu) = \iint \frac{\varphi_{\varepsilon,s}(x)e^{-\lambda|x-y|}}{4\pi|x-y|}d\mu(y) d\mu(x) = \int \varphi_{\varepsilon,s}(x)V_{\lambda,\mu}(x)d\mu(x)$$

To show that this leads to (4.13) we use the Lax-Milgram theorem [Eva22, Chapter 6.2.1, Theorem 1]. For any $\lambda > 0$ define the bilinear, or better sesquilinear, form

$$B[\cdot,\cdot]:H^1\times H^1\to\mathbb{R},\quad (u,v)\mapsto B[u,v]:=\langle\nabla u,\nabla v\rangle_{L^2}+\lambda^2\langle u,v\rangle_{L^2}.$$

Then B is coercive and bounded (with respect to the H^1 norm) and thus fulfills the conditions of the Lax-Milgram Theorem. Let

$$f(\cdot): H^1 \to \mathbb{C}, \quad g \mapsto f(g) := \int_{\mathbb{R}^3} g(x) d\mu(x)$$

for $\mu \in H^{-1}$ a bounded measure. Then f is a bounded linear functional on H^1 and by the Lax-Milgram theorem there exists a unique $v_0 \in H^1$ such that

$$\int_{\mathbb{R}^3} g d\mu = f(g) = B[g, v_0] = \langle \nabla g, \nabla v_0 \rangle_{L^2} + \lambda^2 \langle g, v_0 \rangle_{L^2}. \tag{4.17}$$

Recall that this solution v_0 is the weak solution of Equation (4.10), hence

$$\int_{\mathbb{R}^3} g d\mu = \langle \nabla g, \nabla V_{\mu,\lambda} \rangle_{L^2} + \lambda^2 \langle g, V_{\mu,\lambda} \rangle_{L^2}. \tag{4.18}$$

for all $g \in H^1(\mathbb{R}^3)$. Using $g = \varphi_{\varepsilon,s} V_{\lambda,\mu}$ proves

$$\frac{1}{4\pi}I_{s}^{\lambda,\varepsilon}(\mu,\mu) = \int \varphi_{\varepsilon,s}V_{\lambda,\mu}d\mu = \left\langle \nabla(\varphi_{\varepsilon,s}V_{\lambda,\mu}), \nabla V_{\lambda,\mu} \right\rangle + \lambda \left\langle \varphi_{\varepsilon,s}V_{\lambda,\mu}, V_{\lambda,\mu} \right\rangle$$

which is (4.13).

5. Mean-Field type bounds

In this section we analyze $\alpha_{N,s}$ defined in equation (3.9) and derive lower bounds for $\alpha_{N,s}$ in terms of its mean–field version β_s . Clearly, the quotient in the definition of $\alpha_{N,s}$ is infinite when two points coincide. So let

$$A := \{(x_1, x_2, \dots x_N) \in \mathbb{R}^{3N} : x_i \neq x_j \text{ whenever } i \neq j\}$$

then

$$\alpha_{N,s} = \inf \left\{ \frac{\sum_{1 \le i,k \le N} \frac{|x_k|^s + |x_i|^s}{|x_i - x_k|}}{2(N-1) \sum_{k=1}^N |x_k|^{s-1}} : (x_1, x_2, \dots x_N) \in A \right\}.$$
(5.1)

Note that the mapping

$$(x_1, x_2, \dots x_N) \mapsto \frac{\sum_{1 \le i,k \le N} \frac{|x_k|^s + |x_i|^s}{|x_i - x_k|}}{2(N-1) \sum_{k=1}^N |x_k|^{s-1}}$$

is continuous on A. The set

$$A_0 := \{(x_1, x_2, \dots x_N) \in A : x_k \neq 0 \text{ for } 1 \le k \le N\}$$
 (5.2)

is dense in A thus

$$\alpha_{N,s} = \inf \left\{ \frac{\sum_{1 \le j,k \le N} \frac{|x_j|^s + |x_k|^s}{|x_i - x_k|}}{2(N-1) \sum_{k=1}^N |x_k|^{s-1}} : (x_1, x_2, \dots x_N) \in A_0 \right\}.$$
 (5.3)

For completeness we prove this in the Appendix in Lemma A.1. In order to prove that $\alpha_{N,s} \to \beta_s$ for $N \to \infty$, with β_s given by (4.1) we need some preparations.

Lemma 5.1. Let r > 0, $x \in \mathbb{R}^3 \setminus \{0\}$ and μ be the measure defined by

$$\int_{\mathbb{R}^3} f d\mu := \int_{S^2} f(x + r |x| \omega) \frac{d\omega}{4\pi}$$
 (5.4)

for any measurable function f. Then $\mu \in H^{-1}(\mathbb{R}^3)$.

Remark 5.2. This lemma shows that convex combinations of probability measures of the form (5.4) are allowed in the computation of upper bounds for β_s since they clearly are in $P(\mathbb{R}^3) \cap M_{s-1}(\mathbb{R}^3)$ and the lemma shows that they are also in $H^{-1}(\mathbb{R}^3)$.

Proof. Let r > 0, $\Omega := \{x \in \mathbb{R}^3 : |x| < r\}$ and $T : H^1(\Omega) \to L^2(\partial\Omega)$ the trace operator as for example defined in [Eva22, Chapter 5.5]. Furthermore, let $f \in H^1(\mathbb{R}^3)$ then

$$\left| \int_{\mathbb{R}^3} f d\mu \right| = \left| \int_{S^2} f(x + r |x| \omega) \frac{d\omega}{4\pi} \right| \le \frac{1}{4\pi} \int_{\partial\Omega} |(Tf)(\omega)| d\omega \le r^{1/2} ||Tf||_{L^2(\partial\Omega)}.$$

The Trace Theorem [Eva22, Chapter 5.5 Theorem 1] shows that there exists a C>0 such that

$$\|Tf\|_{L^2(\partial\Omega)} \leq C \, \|f\|_{H^1(\Omega)} < \infty \, .$$

Consequently, μ is in the dual space of $H^1(\mathbb{R}^3)$ by definition of the dual space. That is, $\mu \in H^{-1}(\mathbb{R}^3)$.

We continue by comparing $\alpha_{N,s}$ to β_s . Let r > 0 and $(x_1, ..., x_N) \in \mathbb{R}^{3N}$ with $x_j \neq x_k$ for $j \neq k$. Following [Nam12] we define

$$\mu := \frac{1}{N} \sum_{i=1}^{N} d\mu_i, \int_{\mathbb{R}^3} f d\mu_i := \int_{S^2} f(x_j + r \left| x_j \right| \omega) \frac{d\omega}{4\pi}$$
 (5.5)

for any measurable function f. By Lemma 5.1 $x_i \neq 0$ implies that $\mu_i \in H^{-1}$. In our analysis, we will use a refinement of the following Lemma 5.3. We provide this bound, since it allows to compare $\alpha_{N,s}$ and β_s for all s > 0 and large N, while the refinements only work for $s \geq 2$.

Lemma 5.3 (Comparison of $\alpha_{N,s}$ with β_s , all $s \ge 0$). Let $\alpha_{N,s}$ and β_s be defined as in (4.1) and (5.1) then for every $N \ge 2$, r > 0, and $s \ge 0$

$$\frac{(r+1)^{s+1} - (1-r)^{s+1}}{2r(s+1)} N\beta_s \le (1+r)^s \left(\alpha_{N,s}(N-1) + \frac{1}{r}\right)$$
(5.6)

Remark 5.4. Note that the prefactors in front of $N\beta_s$ and $\alpha_{N,s}(N-1)$ in (5.6) converges to one as $r \to 0$. Thus (5.6) shows that for all r > 0

$$\liminf_{N\to\infty} \alpha_{N,s} \geq \frac{(1+r)^{s+1} - (1-r)^{s+1}}{2r(s+1)(1+r)^s} \beta_s.$$

Taking the limit $r \to 0$ yields $\liminf_{N \to \infty} \alpha_{N,s} \ge \beta_s$ and with Lemma 3.3 this proves

$$\lim_{N\to\infty}\alpha_{N,s}=\beta_s$$

for all s > 0.

Proof of Lemma 5.3. Let $\mu = \sum_{j=1}^{N} \mu_j$ for points $x_1, \ldots, x_N \in A_0$, where A_0 is defined in (5.2), be the measure given by (5.5). By Lemma 5.1 we know that $\mu \in H^{-1}(\mathbb{R}^3)$. Recall the definition of I_s in Lemma 4.3. Then

$$N^{2}I_{s}(\mu) = \sum_{j,k=1}^{N} \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\mu_{j}(x) d\mu_{k}(y)$$

$$= \sum_{j \neq k}^{N} \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\mu_{j}(x) d\mu_{k}(y)$$

$$+ \sum_{j=1}^{N} \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\mu_{j}(x) d\mu_{j}(y)$$
(5.7)

Note that by construction of the measure μ_i

$$|x - x_i| = r |x_i|$$

and hence

$$|x| \le |x - x_i| + |x_i| \le (1 + r) |x_i|.$$
 (5.8)

for any $x \in \text{supp}(\mu_i)$. We first bound the diagonal terms with j = k. Note that

$$\iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\mu_{j}(x) d\mu_{j}(y) = \int_{\mathbb{R}^{3}} |x|^{s} \int_{\mathbb{R}^{3}} \frac{1}{|x - y|} d\mu_{j}(y) d\mu_{j}(x)
\leq (1 + r)^{s} |x_{i}|^{s} \int_{\mathbb{R}^{3}} \int_{S^{2}} \frac{1}{|x - x_{j} - r| |x_{i}| |\omega|} \frac{d\omega}{4\pi} d\mu_{i}(x)
= (1 + r)^{s} |x_{j}|^{s} \int_{S^{2}} \int_{S^{2}} \frac{1}{|r| |x_{j}| |\eta - r| |x_{j}| |\omega|} \frac{d\omega}{4\pi} \frac{d\eta}{4\pi}
= \frac{|x_{j}|^{s-1}}{r} (1 + r)^{s}.$$
(5.9)

Hence

$$\sum_{j=1}^{N} \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\mu_{j}(x) d\mu_{j}(y) \le \frac{(1 + r)^{s}}{r} \sum_{j=1}^{N} |x_{j}|^{s-1}.$$
(5.10)

Similarly, we can bound the off-diagonal terms $j \neq k$. We have

$$\iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\mu_{j}(x) d\mu_{k}(y)
= \int_{\mathbb{R}^{3}} |x|^{s} \int_{\mathbb{R}^{3}} \frac{1}{|x - y|} d\mu_{k}(y) d\mu_{j}(x)
\leq (1 + r)^{s} |x_{j}|^{s} \int_{\mathbb{R}^{3}} \int_{S^{2}} \frac{1}{|x - x_{k} - r| |x_{k}| |\omega|} \frac{d\omega}{4\pi} d\mu_{j}(x)
= (1 + r)^{s} |x_{j}|^{s} \int_{\mathbb{R}^{3}} \frac{1}{\max\{|x - x_{j}|, r|x_{j}|\}} d\mu_{j}(x)
\leq (1 + r)^{s} |x_{i}|^{s} \int_{\mathbb{R}^{3}} \frac{1}{|x - x_{i}|} d\mu_{j}(x) \leq (1 + r)^{s} \frac{|x_{i}|^{s}}{|x_{i} - x_{i}|}.$$
(5.11)

Thus

$$\sum_{j \neq k} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x - y|} d\mu_j(x) d\mu_k(y) \le (1 + r)^s \sum_{j \neq k}^N \frac{|x_j|^s + |x_k|^s}{2|x_j - x_k|}.$$
 (5.12)

Combining (5.7), (5.9) and (5.12) shows

$$N^{2}I_{s}(\mu) \leq \frac{(1+r)^{s}}{r} \sum_{j=1}^{N} \left| x_{j} \right|^{s-1} + (1+r)^{s} \sum_{j\neq k}^{N} \frac{\left| x_{j} \right|^{s} + \left| x_{k} \right|^{s}}{2\left| x_{j} - x_{k} \right|}.$$
 (5.13)

Let t > -2 then with Lemma A.3 we have

$$N \int_{\mathbb{R}^3} |x|^t d\mu = \sum_{j=1}^N \int_{S^2} |x_j + r| x_j |\omega|^t \frac{d\omega}{4\pi} = \frac{(1+r)^{t+2} - (1-r)^{t+2}}{2r(t+2)} \sum_{j=1}^N |x_j|^t . \tag{5.14}$$

Applying (5.14) for t = s - 1 yields

$$N \int_{\mathbb{R}^3} |x|^{s-1} d\mu(x) = \frac{(1+r)^{s+1} - (1-r)^{s+1}}{2r(s+1)} \sum_{j=1}^N |x_j|^{s-1}.$$
 (5.15)

Recall the definitions of β_s and $I_s(\mu)$ in (4.1) and (4.4) then $\beta_s \leq I_s(\mu)/\int |x|^{s-1} d\mu$ or

$$N \int_{\mathbb{R}^3} |x|^{s-1} d\mu(x) \, \beta_s N \le N^2 I_s(\mu) \,, \tag{5.16}$$

which together with (5.13) and (5.15) implies the inequality

$$\frac{(1+r)^{s+1} - (1-r)^{s+1}}{2r(s+1)(1+r)^s} \beta_s N \le \frac{1}{r} + \frac{\sum_{j \neq k} \frac{\left|x_j\right|^s + |x_k|^s}{2|x_j - x_k|}}{\sum_{j=1}^N \left|x_j\right|^{s-1}}$$

Taking the infimum in the positions $(x_1, x_2, ..., x_N) \in A_0$ together with the definition of $\alpha_{N,s}$ and applying Lemma A.1 we conclude

$$\frac{(1+r)^{s+1}-(1-r)^{s+1}}{2r(s+1)(1+r)^s}\beta_s N \leq \frac{1}{r}+\alpha_{N,s}(N-1).$$

This proves (5.6).

Lemma 5.5 (Refined comparison I of $\alpha_{N,s}$ with β_s , $s \ge 2$). For $s \ge 2$ and all $N \in \mathbb{N}$ and r > 0 we have

$$\left(\frac{s+2}{s+1}\right) \frac{(1+r)^{s+1} - |1-r|^{s+1}}{(1+r)^{s+2} - |1-r|^{s+2}} N\beta_s - \frac{1}{r} \le \frac{2r(s+2)}{(1+r)^{s+2} - |1-r|^{s+2}} g(r) \alpha_{N,s}(N-1) .$$
(5.17)

where

$$g(r) = (1+r^2)^{s/2} \left(\frac{(1+q)^{s/2} + (1-q)^{s/2}}{2} - \frac{s(s-2)}{15} q^2 (1+q)^{\frac{s-4}{2}} \right), \quad q = \frac{2r}{1+r^2}. \quad (5.18)$$

Remark 5.6. For s = 2, the bound (5.17) is similar to the refined bound (27) in [Nam12]. The main challenge in establishing a relationship between $\alpha_{N,s}$ and β_s arises from the weighted Coulomb interaction term in (5.11). In the proof of Lemma 5.5, we improve the estimate of these terms using a convexity argument.

Since obtaining optimal estimates between $\alpha_{N,s}$ and β_s is technically challenging, we present the proof of Lemma 5.5 here, relying on convexity. A further refinement is provided in Lemma 5.9. This improvement, which is more difficult to prove as it involves a multipole expansion and estimates for all multipole moments using certain nontrivial properties of Legendre polynomials, yields a better constant in front of $\beta_s N$.

Before we give the proof of Lemma 5.5, we state and prove a result which is extremely helpful dropping certain terms when deriving a bound on $\alpha_{N,s}$ in terms of β_s when $s \ge 2$.

Lemma 5.7. Let $\gamma:(0,\infty)\times(0,\infty)\to[0,\infty)$ a function such that $\gamma(u,v)$ is increasing in v for any fixed u>0. Then for any N dinstinct points x_1,\ldots,x_N in $\mathbb{R}^3\setminus\{0\}$ we have

$$\sum_{j \neq k} \frac{\gamma(\left|x_{j} - x_{k}\right|, r\left|x_{j}\right|)}{\left|x_{j}\right|} x_{j} \cdot (x_{j} - x_{k}) \ge 0$$

$$(5.19)$$

for all r > 0

Proof. Since the sum is over pais $j \neq k$ it is enough to consider the case N=2 and i=1, j=2. Set $a=x_1-x_2$. We have $x_1\cdot(x_1-x_2)=|x_1|^2-x_1\cdot x_2\geq |x_1|^2-|x_1|\,|x_2|$ and, similarly, $x_2\cdot(x_2-x_1)\geq |x_2|^2-|x_2|\,|x_1|$. Since $\gamma\geq 0$ $\gamma(|a|,v_1)\geq \gamma(|a|,v_2)$ if $v_1\geq v_2$, by assumption this implies

$$\frac{\gamma(|x_{1}-x_{2}|,r|x_{1}|)}{|x_{1}|}x_{1} \cdot (x_{1}-x_{2}) + \frac{\gamma(|x_{2}-x_{1}|,r|x_{2}|)}{|x_{2}|}x_{2} \cdot (x_{2}-x_{1})$$

$$\geq \gamma(|a|,r|x_{1}|) (|x_{1}|-|x_{2}|) + \gamma(|a|,r|x_{2}|) (|x_{2}|-|x_{1}|)$$

$$= (\gamma(|a|,r|x_{1}|) - \gamma(|a|,r|x_{2}|)) (|x_{1}|-|x_{2}|) \geq 0.$$

Remark 5.8. We note that unlike the proof in [Nam12], we do not need the explicit form of $\gamma(u, v)$ in (5.35) for (5.19). Our argument shows that it is enough that $\gamma(u, v) \geq 0$ is increasing in v > 0 for fixed u > 0.

Proof of Lemma 5.5. The diagonal terms are easy to calculate. Without loss of generality, let j = 1. Then by symmetry, the definition of the measures μ_j , and Newton's theorem we have

$$\iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\mu_{1}(x) d\mu_{1}(y) = \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s}}{|x - y|} d\mu_{1}(x) d\mu_{1}(y)
= \frac{1}{(4\pi)^{2}} \int_{S^{2}} \int_{S^{2}} \frac{|x_{1} + r|x_{1}| \omega_{1}|^{s}}{|r|x_{1}| |\omega_{1} - \omega_{2}|} d\omega_{1} d\omega_{2} = \frac{1}{4\pi r |x_{1}|} |x_{1}|^{s-1} \int_{S^{2}} |\widehat{x}_{1} + r\omega|^{s} d\omega \quad (5.20)
= \frac{|x_{1}|^{s-1}}{r} \frac{(1+r)^{s+2} - |1-r|^{s+2}}{2r(s+2)}.$$

See Lemma A.3 for the explicit calculation of the last integral in (5.20). Thus the diagonal sum is given by

$$\sum_{j=1}^{N} \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x-y|} d\mu_{j}(x) d\mu_{k}(y) = \frac{(1+r)^{s+2} - |1-r|^{s+2}}{2r^{2}(s+2)} \sum_{j=1}^{N} |x_{j}|^{s-1} . \tag{5.21}$$

For the off-diagonal sum we use symmetry and Newton's theorem – the measure μ_j is radially symmetric around the point x_j – to see that

$$\sum_{j \neq k} \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\mu_{j}(x) d\mu_{k}(y) = \sum_{j \neq k} \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s}}{|x - y|} d\mu_{k}(y) d\mu_{j}(x)$$

$$\leq \sum_{j \neq k} \int_{\mathbb{R}^{3}} \frac{|x|^{s}}{|x - x_{j}|} d\mu_{j}(x) = \sum_{j \neq k} \frac{1}{4\pi} \int_{S^{2}} \frac{|x_{j} + r|x_{j}|\omega|^{s}}{|x_{j} - x_{k} + r|x_{j}|\omega|} d\omega$$
(5.22)

To bound the integral in the last sum for $s \neq 2$ the estimates presented in [Nam12, Section 4] can not easily be applied, we will proceed differently. With $\hat{x} = x/|x|$ for $x \in \mathbb{R}^3 \setminus \{0\}$ and $q = 2r/(1+r^2)$ we have for the numerator in the last term of (5.22)

$$|x_j + r|x_j|\omega|^s = |x_j|^s (\hat{x}_j + r\omega)^s = |x_j|^s (1 + r^2 + 2r\hat{x}_j \cdot \omega)^{s/2} = |x_j|^s (1 + r^2)^{s/2} (1 + q\hat{x}_j \cdot \omega)^{s/2}.$$
(5.23)

Set for $t \in [-1, 1]$ and $d \in \mathbb{R}$

$$F(t) := (1+qt)^{s/2}, \quad H_d(t) := F(t) - d(t^2 - 1)$$
 (5.24)

We determine $d \in \mathbb{R}$ depending on $q, s \in \mathbb{R}$ such that H is convex. Note that $H''_d = F'' - 2d$. Consequently to ensure convexity of H_d we need

$$d \le \frac{1}{2}F''(t) = \frac{s}{4} \left(\frac{s}{2} - 1\right) q^2 (1 + qt)^{\frac{s-4}{2}} \le \frac{s}{4} \left(\frac{s}{2} - 1\right) q^2 (1 + qt)^{\frac{s-4}{2}}$$

We fix

$$d_0 := \frac{s}{4} \left(\frac{s}{2} - 1 \right) q^2 (1 + q)^{\frac{s-4}{2}} \tag{5.25}$$

such that H_{d_0} is convex. Due to the convexity of H_{d_0} we have

$$H_{d_0}(t) \leq \frac{H_{d_0}(1) - H_{d_0}(-1)}{2} t + \frac{H_{d_0}(1) + H_{d_0}(-1)}{2} \,.$$

Since $H_{d_0} = F(t) - d_0(t^2 - 1)$ this yields

$$F(t) \le \frac{F(1) - F(-1)}{2}t + \frac{F(1) + F(-1)}{2} + d_0(t^2 - 1)$$
(5.26)

Inserting $F(t) = (1 + qt)^{s/2}$ and d_0 from (5.25) into (5.26) we arrive at

$$(1+qt)^{s/2} \le \frac{(1+q)^{s/2} - (1-q)^{s/2}}{2}t + \frac{(1+q)^{s/2} + (1-q)^{s/2}}{2} + \frac{s}{4}\left(\frac{s}{2} - 1\right)q^2(1+q)^{\frac{s-4}{2}}(t^2 - 1)$$
(5.27)

Combining (5.22), (5.23) and (5.27) yields

$$\sum_{j \neq k} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x - y|} d\mu_j(x) d\mu_k(y)$$

$$\leq (1+r^{2})^{s/2} \frac{(1+q)^{s/2} - (1-q)^{s/2}}{2} \sum_{j\neq k} |x_{j}|^{s} \int_{S^{2}} \frac{\hat{x}_{j} \cdot \omega}{|x_{j} - x_{k} + r|x_{j}| \omega|} \frac{d\omega}{4\pi} \\
+ (1+r^{2})^{s/2} \frac{(1+q)^{s/2} + (1-q)^{s/2}}{2} \sum_{j\neq k} |x_{j}|^{s} \int_{S^{2}} \frac{1}{|x_{j} - x_{k} + r|x_{j}| \omega|} \frac{d\omega}{4\pi} \\
+ (1+r^{2})^{s/2} \frac{s}{4} \left(\frac{s}{2} - 1\right) q^{2} (1+q)^{\frac{s-4}{2}} \sum_{j\neq k} |x_{j}|^{s} \int_{S^{2}} \frac{(\hat{x}_{j} \cdot \omega)^{2} - 1}{|x_{j} - x_{k} + r|x_{j}| \omega|} \frac{d\omega}{4\pi}$$
(5.28)

We proceed by estimating each of the summands in the right-hand side of (5.28) independently. We begin by showing that the first summand is negative. Let $a_{jk} := (x_k - x_j)/|x_j|$ then

$$\left|x_{j}\right|^{s} \int_{S^{2}} \frac{\hat{x}_{j} \cdot \omega}{\left|x_{j} - x_{k} + r\left|x_{j}\right|\omega\right|} \frac{d\omega}{4\pi} = \left|x_{j}\right|^{s-1} \int_{S^{2}} \frac{\hat{x}_{j} \cdot \omega}{\left|a_{jk} - r\omega\right|} \frac{d\omega}{4\pi}$$
(5.29)

which either can be solved in polar coordinates directly or using multipol expansion, that is expanding the Coulomb–kernel in terms of the Legendre Polynomials $P_l(t)$, $l \in \mathbb{N}_0$. Using the generating function

$$(1 + \delta^2 - 2\delta t)^{-1/2} = \sum_{n=0}^{\infty} \delta^n P_n(t)$$
 (5.30)

which is valid for $|t| \le 1$ and $|\delta| < 1$. We can always assume that $r \ne |a_{jk}|$ since otherwise we replace r with $r_{\varepsilon} = r + \varepsilon$ and take the limit $\varepsilon \to 0$ after solving the integral. Expanding $|a_{jk} - r\omega|^{-1}$ yields

$$\left| a_{jk} - r\omega \right|^{-1} = \sum_{n=0}^{\infty} \frac{\min\{\left| a_{jk} \right|, r\}^n}{\max\{\left| a_{jk} \right|, r\}^{n+1}} P_n(\omega \cdot \hat{a}_{jk})$$
 (5.31)

Using $P_1(\hat{x}_j \cdot \omega) = \hat{x}_j \cdot \omega$ and inserting (5.31) into (5.29) we arrive at

$$|x_{j}|^{s} \int_{S^{2}} \frac{\hat{x}_{j} \cdot \omega}{|x_{j} - x_{k} + r|x_{j}| \omega} \frac{d\omega}{4\pi} = |x_{j}|^{s-1} \int_{S^{2}} \sum_{n=0}^{\infty} \frac{\min\{|a_{jk}|, r\}^{n}}{\max\{|a_{jk}|, r\}^{n+1}} P_{n}(\omega \cdot \hat{a}_{jk}) P_{1}(\hat{x}_{j} \cdot \omega) \frac{d\omega}{4\pi}$$

$$= |x_{j}|^{s-1} \sum_{n=0}^{\infty} \frac{\min\{|a_{jk}|, r\}^{n}}{\max\{|a_{jk}|, r\}^{n+1}} \int_{S^{2}} P_{n}(\omega \cdot \hat{a}_{jk}) P_{1}(\hat{x}_{j} \cdot \omega) \frac{d\omega}{4\pi}$$
(5.32)

Legendre Polynomials are orthogonal in the following sense

$$\int_{-1}^{1} P_n(t) P_m(t) dt = \frac{2\delta_{mn}}{2n+1},$$
(5.33)

and consequently by the Funk-Hecke formula in Lemma A.3 we arrive at

$$\int_{S^2} P_n(\hat{x}_j \cdot \omega) P_m(\omega \cdot \hat{a}_{jk}) \, \frac{d\omega}{4\pi} = \frac{\delta_{mn}}{2n+1} \,. \tag{5.34}$$

Inserting (5.34) into (5.32) we arrive at

$$\begin{aligned} |x_{j}|^{s} \int_{S^{2}} \frac{\hat{x}_{j} \cdot \omega}{|x_{j} - x_{k} + r|x_{j}| \omega|} \frac{d\omega}{4\pi} &= |x_{j}|^{s-1} \frac{\min\{|a_{jk}|, r\}}{\max\{|a_{jk}|, r\}^{2}} \frac{\hat{a}_{jk} \cdot \hat{x}_{j}}{3} \\ &= -|x_{j}|^{s-1} \frac{\min\{|a_{jk}|, r\}}{\max\{|a_{jk}|, r\}^{2}} \frac{(x_{j} - x_{k}) \cdot \hat{x}_{j}}{3|x_{k} - x_{j}|} \\ &= -|x_{j}|^{s} \frac{\min\{|x_{j} - x_{k}|, r|x_{j}|\}}{\max\{|x_{j} - x_{k}|, r|x_{j}|\}^{2}} \frac{1}{3|x_{k} - x_{j}|} (x_{j} - x_{k}) \cdot \hat{x}_{j} \\ &= -r^{-s} \gamma \left(|x_{j} - x_{k}|, r|x_{j}|\right) (x_{j} - x_{k}) \cdot \hat{x}_{j} \end{aligned}$$

with

$$\gamma(u,v) = \frac{v^{s} \min(u,v)}{3u \max(u,v)^{2}}.$$
(5.35)

for u, v > 0. Summing (5.32) over $j \neq k$ yields

$$\sum_{j\neq k} \left| x_j \right|^s \int_{S^2} \frac{\hat{x}_j \cdot \omega}{\left| x_j - x_k + r \left| x_j \right| \omega \right|} \frac{d\omega}{4\pi} = -r^{-s} \sum_{j\neq k} \gamma \left(\left| x_j - x_k \right|, r \left| x_j \right| \right) \left(x_j - x_k \right) \cdot \hat{x}_j \tag{5.36}$$

Applying Lemma 5.7 and noting Remark 5.8 we find

$$\sum_{j\neq k} \gamma(\left|x_{j}-x_{k}\right|, r\left|x_{j}\right|) \widehat{x}_{j} \cdot \left(x_{j}-x_{k}\right) \geq 0.$$

Thus the first summand in the right-hand side of (5.28) is not positive and consequently

$$\sum_{j\neq k} \iint_{\mathbb{R}^{3}\times\mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\mu_{j}(x) d\mu_{k}(y)
\leq (1 + r^{2})^{s/2} \frac{(1 + q)^{s/2} + (1 - q)^{s/2}}{2} \sum_{j\neq k} |x_{j}|^{s} \int_{S^{2}} \frac{1}{|x_{j} - x_{k} + r|x_{j}|\omega|} \frac{d\omega}{4\pi}
+ (1 + r^{2})^{s/2} \frac{s}{4} \left(\frac{s}{2} - 1\right) q^{2} (1 + q)^{\frac{s-4}{2}} \sum_{j\neq k} |x_{j}|^{s} \int_{S^{2}} \frac{(\hat{x}_{j} \cdot \omega)^{2} - 1}{|x_{j} - x_{k} + r|x_{j}|\omega|} \frac{d\omega}{4\pi}$$
(5.37)

The first integral in the right-hand side of (5.37) can be solved since due to Newton's theorem

$$\int_{S^2} \frac{1}{|x_j - x_k + r| |x_j| |\omega|} \frac{d\omega}{4\pi} = \frac{1}{\max\{|x_j - x_k|, r|x_j|\}}.$$
 (5.38)

Inserting (5.38) into (5.37) yields

$$\sum_{j \neq k} \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\mu_{j}(x) d\mu_{k}(y)
\leq (1 + r^{2})^{s/2} \frac{(1 + q)^{s/2} + (1 - q)^{s/2}}{2} \sum_{j \neq k} \frac{|x_{j}|^{s}}{\max\{|x_{j} - x_{k}|, r |x_{j}|\}}
+ (1 + r^{2})^{s/2} \frac{s}{4} \left(\frac{s}{2} - 1\right) q^{2} (1 + q)^{\frac{s-4}{2}} \sum_{j \neq k} |x_{j}|^{s} \int_{S^{2}} \frac{(\hat{x}_{j} \cdot \omega)^{2} - 1}{|x_{j} - x_{k}| + r |x_{j}| \omega|} \frac{d\omega}{4\pi} .$$
(5.39)

Next we estimate the remaining integral in the right-hand side of (5.39), in particular we aim to solve

$$|x_{j}|^{s} \int_{S^{2}} \frac{(\hat{x}_{j} \cdot \omega)^{2} - 1}{|x_{j} - x_{k} + r|x_{j}|\omega|} \frac{d\omega}{4\pi} = |x_{j}|^{s-1} \int_{S^{2}} \frac{(\hat{x}_{j} \cdot \omega)^{2} - 1}{|a_{jk} - r\omega|} \frac{d\omega}{4\pi}$$
(5.40)

We use

$$\frac{2}{3}P_2(t) - \frac{2}{3} = t^2 - 1, \quad \forall t \in [-1, 1], \tag{5.41}$$

where P_2 is the second-order Legendre polynomial. Inserting (5.41) into (5.40) we find

$$|x_{j}|^{s} \int_{S^{2}} \frac{(\hat{x}_{j} \cdot \omega)^{2} - 1}{|x_{j} - x_{k} + r|x_{j}|\omega|} \frac{d\omega}{4\pi} = \frac{2}{3} |x_{j}|^{s-1} \int_{S^{2}} \frac{P_{2}(\hat{x}_{j} \cdot \omega) - 1}{|a_{jk} - r\omega|} \frac{d\omega}{4\pi}$$

$$= \frac{2}{3} |x_{j}|^{s-1} \left(\int_{S^{2}} \frac{P_{2}(\hat{x}_{j} \cdot \omega)}{|a_{jk} - r\omega|} \frac{d\omega}{4\pi} - \frac{1}{\max\{|a_{jk}|, r\}} \right).$$
(5.42)

where we have used Newton's theorem. To solve the integral involving the Legendre polynomial P_2 we use the multipol expansion in (5.31) and (5.34) to find

$$\int_{S^{2}} \frac{P_{2}(\hat{x}_{j} \cdot \omega)}{|a_{jk} - r\omega|} \frac{d\omega}{4\pi} = \sum_{n=0}^{\infty} \frac{\min\{|a_{jk}|, r\}^{n}}{\max\{|a_{jk}|, r\}^{n+1}} \int_{S^{2}} P_{n}(\omega \cdot \hat{a}_{jk}) P_{2}(\hat{x}_{j} \cdot \omega) \frac{d\omega}{4\pi}
= \frac{\min\{|a_{jk}|, r\}^{2}}{\max\{|a_{jk}|, r\}^{3}} \frac{P_{2}(\hat{a}_{jk} \cdot \omega)}{5} \leq \frac{1}{5 \max\{|a_{jk}|, r\}}$$
(5.43)

Using $\left|a_{jk}\right| = \left|x_j - x_k\right| / \left|x_j\right|$ and inserting (5.43) into (5.42) shows

$$|x_{j}|^{s} \int_{S^{2}} \frac{(\hat{x}_{j} \cdot \omega)^{2} - 1}{|x_{j} - x_{k} + r|x_{j}|\omega|} \frac{d\omega}{4\pi} \le \frac{-8}{15} \frac{|x_{j}|^{s}}{\max\{|x_{j} - x_{k}|, r|x_{j}|\}}.$$
 (5.44)

Combining (5.39) and (5.44) we arrive at

$$\sum_{j\neq k} \iint_{\mathbb{R}^{3}\times\mathbb{R}^{3}} \frac{|x|^{s} + |y|^{s}}{2|x - y|} d\mu_{j}(x) d\mu_{k}(y)$$

$$\leq (1 + r^{2})^{s/2} \frac{(1 + q)^{s/2} + (1 - q)^{s/2}}{2} \sum_{j\neq k} \frac{|x_{j}|^{s}}{\max\{|x_{j} - x_{k}|, r |x_{j}|\}}$$

$$- \frac{8}{15} (1 + r^{2})^{s/2} \frac{s}{4} \left(\frac{s}{2} - 1\right) q^{2} (1 + q)^{\frac{s-4}{2}} \sum_{j\neq k} \frac{|x_{j}|^{s}}{\max\{|x_{j} - x_{k}|, r |x_{j}|\}}$$

$$= (1 + r^{2})^{s/2} \left(\frac{(1 + q)^{s/2} + (1 - q)^{s/2}}{2} - \frac{s (s - 2)}{15} q^{2} (1 + q)^{\frac{s-4}{2}}\right) \sum_{j\neq k} \frac{|x_{j}|^{s}}{\max\{|x_{j} - x_{k}|, r |x_{j}|\}}$$

$$= \underbrace{(1 + r^{2})^{s/2} \left(\frac{(1 + q)^{s/2} + (1 - q)^{s/2}}{2} - \frac{s (s - 2)}{15} q^{2} (1 + q)^{\frac{s-4}{2}}\right)}_{=:q(r)} \sum_{j\neq k} \frac{|x_{j}|^{s}}{\max\{|x_{j} - x_{k}|, r |x_{j}|\}}$$

Using $q = 2r/(1+r^2)$ one checks by direct computations that $g(r) \ge 0$. Consequently we find

$$\sum_{j \neq k} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x - y|} d\mu_j(x) d\mu_k(y) \le g(r) \sum_{j \neq k} \frac{|x_j|^s + |x_k|^s}{2|x_j - x_k|}$$
(5.45)

Combining the estimates of the diagonal terms (5.20) and the off-diagonal terms (5.45) together with (5.7) yields

$$N^{2}I_{s}(\mu) \leq \frac{(1+r)^{s+2} - |1-r|^{s+2}}{2r^{2}(s+2)} \sum_{j=1}^{N} \left| x_{j} \right|^{s-1} + g(r) \sum_{j \neq k} \frac{\left| x_{j} \right|^{s} + \left| x_{k} \right|^{s}}{2\left| x_{j} - x_{k} \right|}$$
(5.46)

Applying Lemma A.3 we also get

$$N\int |x|^{s-1} d\mu(x) = \sum_{j=1}^{N} |x|^{s-1} d\mu_j(x) = \frac{(1+r)^{s+1} - |1-r|^{s+1}}{2r(s+1)} \sum_{j=1}^{N} |x_j|^{s-1} .$$
 (5.47)

Combining (5.46) and (5.47) shows

$$N\beta_{s} \leq \frac{N^{2}I_{s}(\mu)}{N\int |x|^{s-1}d\mu(x)}$$

$$\leq \frac{1}{r}\left(\frac{s+1}{s+2}\right)\frac{(1+r)^{s+2} - |1-r|^{s+2}}{(1+r)^{s+1} - |1-r|^{s+1}} + \frac{2r(s+1)g(r)}{(1+r)^{s+1} - |1-r|^{s+1}} \frac{\sum\limits_{1\leq j< k\leq N} \frac{|x_{j}|^{s} + |x_{k}|^{s}}{2|x_{j} - x_{k}|}}{\sum\limits_{i=1}^{N} |x_{i}|^{s-1}}.$$

$$(5.48)$$

Taking the infimum over the positions $x_1, x_2, \dots x_N \in A_0$ together with the definition of $\alpha_{N,s}$ in (5.3) we conclude from (5.48)

$$N\beta_s \le \frac{1}{r} \left(\frac{s+1}{s+2} \right) \frac{(1+r)^{s+2} - |1-r|^{s+2}}{(1+r)^{s+1} - |1-r|^{s+1}} + \frac{2r(s+1)g(r)}{(1+r)^{s+1} - |1-r|^{s+1}} \alpha_{N,s}(N-1)$$
(5.49)

and equivalently

$$\left(\frac{s+2}{s+1}\right)\frac{(1+r)^{s+1}-|1-r|^{s+1}}{(1+r)^{s+2}-|1-r|^{s+2}}N\beta_s-\frac{1}{r}\leq \frac{2r(s+2)g(r)}{(1+r)^{s+2}-|1-r|^{s+2}}\alpha_{N,s}(N-1)$$

This finishes the proof of Lemma 5.5.

For small r one can find a better bound than the one in Lemma 5.5 by estimating more carefully and not using convexity. But the argument is much more involved. However, since we are interested in bounds for small r > 0, in order to make the prefactor in (5.17) close to one, we will give this improved bound now.

Lemma 5.9 (Refined comparison II of $\alpha_{N,s}$ with β_s , $4 \ge s \ge 2$). Let $\alpha_{N,s}$ and β_s be defined as in (5.1) and (4.1) then for every $N \ge 2$, r > 0, and $4 \ge s \ge 2$

$$\frac{(1+r)^{s+1} - (1-r)^{s+1}}{2r(s+1)} N\beta_s \le \frac{(1+r)^{s+2} - (1-r)^{s+2}}{2r(s+2)} \left(\alpha_{N,s}(N-1) + \frac{1}{r}\right) + r^2 f(r,s)\alpha_{N,s}(N-1) \tag{5.50}$$

with

$$f(r,s) := \frac{s}{2} \left(\frac{s}{2} - 1 \right) \left(\frac{4}{15} + \left(2 - \frac{s}{2} \right) \frac{8}{105} r + \left(2 - \frac{s}{2} \right) \frac{448}{625} r^2 \right). \tag{5.51}$$

In particular, for s = 3 this gives

$$(1+r^2)N\beta_3 - \frac{1+2r^2+r^4/5}{r} \le \alpha_{N,3}(N-1)\left(1+\frac{r^2}{5}+\frac{r^3}{35}+\frac{168}{625}r^4\right). \tag{5.52}$$

Remark 5.10. Note that f(r, 2) vanishes for all r > 0 and for $s \in (2, 3]$ it adds a positive correction to the leading order term in the prefactor of $\alpha_{N,s}$. For later usage, we note that one has the rough estimate $f(r, s) \le f(r, 3) < \frac{1}{2}$ for $r \in [0, 1]$ any $s \in (2, 3]$.

Proof. We again use the bounds (5.7) together with (5.21) and (5.22). In order to improve on Lemma 5.5, we have to bound the integral in the last sum of (5.22) more carefully. Recalling $a_{jk} = (x_k - x_j)/|x_j|$ and $\widehat{x}_j = x_j/|x_j|$ we can rewrite

$$\int_{S^2} \frac{|x_j + r| x_j |\omega|^s}{|x_j - x_k + r| x_j |\omega|} \frac{d\omega}{4\pi} = |x_j|^{s-1} \int_{S^2} \frac{(1 + r^2 + 2r\hat{x}_j \cdot \omega)^{s/2}}{|a_{jk} - r\omega|} \frac{d\omega}{4\pi}$$
(5.53)

Such integrals can be solved by multipole expansion, that is expanding the Coulomb–kernel in terms of the Legendre Polynomials $P_l(t)$, $l \in \mathbb{N}_0$. Using the generating function

$$(1 + \delta^2 - 2\delta t)^{-1/2} = \sum_{n=0}^{\infty} \delta^n P_n(t)$$

which is valid for $|t| \le 1$ and $|\delta| < 1$, and expanding $|a_{jk} - r\omega|^{-1}$ in (5.53) with the help of (5.30) and using Lemma A.2 yields

$$|x_{j}|^{s-1} \int_{S^{2}} \frac{(1+r^{2}+2r\hat{x}_{j}\cdot\omega)^{s/2}}{|a_{jk}-r\omega|} \frac{d\omega}{4\pi}$$

$$=|x_{j}|^{s-1} \sum_{l=0}^{\infty} \frac{\min(|a_{jk}|,r)^{l}}{\max(|a_{jk}|,r)^{l+1}} \int_{S^{2}} (1+r^{2}+2r\hat{x}_{j}\cdot\omega)^{s/2} P_{l}(\langle\hat{a}_{jk},\omega\rangle) \frac{d\omega}{4\pi}$$

$$=|x_{j}|^{s-1} \sum_{l=0}^{\infty} \frac{\min(|a_{jk}|,r)^{l}}{\max(|a_{jk}|,r)^{l+1}} \lambda_{l,s}(r) P_{l}(\hat{a}_{jk}\cdot\hat{x}_{j})$$
(5.54)

with

$$\lambda_{l,s}(r) = \frac{1}{2} \int_{-1}^{1} (1 + r^2 + 2rt)^{s/2} P_l(t) dt.$$

We will see shortly that the sum $\sum_{l=0}^{\infty} \left| \lambda_{l,s}(r) \right|$ converges – see (5.67) – so the series in the last line of (5.54) converges for all r>0 since $-1\leq P_l(t)\leq 1$ for $-1\leq t\leq 1$. Using $P_0(t)\equiv 1$ the first multipole moment l=0 is easy to compute,

$$\lambda_{0,s}(r) = \frac{(1+r)^{s+2} - (1-r)^{s+2}}{2(s+2)r} \,. \tag{5.55}$$

Note that with $P_1(t) = t$ and consequently the second multipole moment is positive non-negative since

$$\lambda_{1,s}(r) = \frac{1}{2} \int_{-1}^{1} (1 + r^2 + 2rt)^{s/2} t dt > 0.$$
 (5.56)

The calculation for higher moments is a bit involved. Before we embark on this, let us note that if $\sum_{l\geq 0} \lambda_{l,s}(r)$ converges absolutely, we can further bound (5.54) as follows.

$$\begin{aligned} \left| x_{j} \right|^{s-1} & \sum_{l=0}^{\infty} \frac{\min(\left| a_{jk} \right|, r)^{l}}{\max(\left| a_{jk} \right|, r)^{l+1}} \lambda_{l,s}(r) P_{l}(\hat{a}_{jk} \cdot \hat{x}_{j}) \\ & \leq \lambda_{0,s}(r) \frac{\left| x_{j} \right|^{s-1}}{\max(\left| a_{jk} \right|, r)} + \lambda_{1,s}(r) \frac{\left| x_{j} \right|^{s-1} \min(\left| a_{jk} \right|, r)}{\max(\left| a_{jk} \right|, r)^{2}} \left(\hat{a}_{jk} \cdot \hat{x}_{j} \right) \\ & + \frac{\left| x_{j} \right|^{s-1}}{\max(\left| a_{jk} \right|, r)} \sum_{l=2}^{\infty} \left| \lambda_{l,s}(r) \right| \end{aligned}$$

Using $a_{jk} = (x_k - x_j)/|x_j|$ we arrive at

$$\begin{aligned} \left| x_{j} \right|^{s-1} & \sum_{l=0}^{\infty} \frac{\min(\left| a_{jk} \right|, r)^{l}}{\max(\left| a_{jk} \right|, r)^{l+1}} \lambda_{l,s}(r) P_{l}(\hat{a}_{jk} \cdot \hat{x}_{j}) \\ & \leq \left(\lambda_{0,s}(r) + \sum_{l=2}^{\infty} \left| \lambda_{l,s}(r) \right| \right) \frac{\left| x_{j} \right|^{s}}{\left| x_{j} - x_{k} \right|} \\ & - \lambda_{1,s}(r) \frac{\left| x_{j} \right|^{s} \min(\left| x_{j} - x_{k} \right|, r \left| x_{j} \right|)}{\left| x_{j} - x_{k} \right| \max(\left| x_{j} - x_{k} \right|, r \left| x_{j} \right|)^{2}} \, \hat{x}_{j} \cdot (x_{j} - x_{k}) \end{aligned}$$

Let $C_s(r) = \sum_{l=2}^{\infty} |\lambda_{l,s}(r)|$ and

$$\widetilde{\gamma}(u,v) = \frac{v^s \min(u,v)}{u \max(u,v)^2}$$

then

$$\begin{aligned} \left| x_{j} \right|^{s-1} & \sum_{l=0}^{\infty} \frac{\min(\left| a_{jk} \right|, r)^{l}}{\max(\left| a_{jk} \right|, r)^{l+1}} \lambda_{l,s}(r) P_{l}(\hat{a}_{jk} \cdot \hat{x}_{j}) \\ & \leq \left(\lambda_{0,s}(r) + C_{s}(r) \right) \frac{\left| x_{j} \right|^{s}}{\left| x_{j} - x_{k} \right|} - \lambda_{1,s}(r) r^{-s} \widetilde{\gamma}(\left| x_{j} - x_{k} \right|, r \left| x_{j} \right|) \hat{x}_{j} \cdot (x_{j} - x_{k}) \end{aligned}$$

Note that $\widetilde{\gamma}(u, v)$ is increasing in v for fixed u > 0. Applying Lemma 5.7 and noting Remark 5.8 we find

$$\sum_{j \neq k} \widetilde{\gamma}(\left|x_{j} - x_{k}\right|, r\left|x_{j}\right|) \widehat{x}_{j} \cdot \left(x_{j} - x_{k}\right) \ge 0.$$
(5.57)

As in (5.22) one sees

$$\sum_{j \neq k} \iint_{\mathbb{R}^{3} \times \mathbb{R}^{3}} \frac{|x|^{s} + |x|^{s}}{2|x - y|} d\mu_{j}(x) d\mu_{k}(y)
\leq \left(\lambda_{0,s}(r) + C_{s}(r)\right) \sum_{j \neq k} \frac{|x_{j}|^{s}}{|x_{j} - x_{k}|} - \lambda_{1,s}(r)r^{-s} \sum_{j \neq k} \widetilde{\gamma}(|x_{j} - x_{k}|, r|x_{j}|) \, \hat{x}_{j} \cdot (x_{j} - x_{k})
\leq \left(\lambda_{0,s}(r) + C_{s}(r)\right) \sum_{j \neq k} \frac{|x_{j}|^{s}}{2|x_{j} - x_{k}|}$$

where we used (5.57) to drop the second sum. In the last line we symmetrized the remaining expression. Thus we get a similar bound as (5.45) with g(r) replaced by $\lambda_{0,s}(r) + C_s(r)$.

Thus, as in the proof of Lemma 5.5, a bound similar to (5.46), but with g(r) in (5.46) replaced by $\lambda_{0,s}(r) + C_s(r)$, follows from this. In particular it follows

$$\left(\frac{s+2}{s+1}\right) \frac{(1+r)^{s+1} - |1-r|^{s+1}}{(1+r)^{s+2} - |1-r|^{s+2}} N\beta_s - \frac{1}{r} \le \left(1 + \frac{2r(s+2)C_s(r)}{(1+r)^{s+2} - |1-r|^{s+2}}\right) \alpha_{N,s}(N-1)$$
(5.58)

Hence the claimed bound (5.50) follows as soon as we can show that

$$C_s(r) \le r^2 f(r, s) \tag{5.59}$$

with f given in (5.51). We will do this in the rest of this proof.

To get a grip on the higher order moments $\lambda_{l,s}(r)$ for $l \geq 2$ we expand $|\hat{x}_j + r\omega|^s$ in a binomial series. With $t = \widehat{x}_j \cdot \omega$ and

$$q = 2r/(1+r^2) \le 1 \tag{5.60}$$

we have

$$(1+r^2+2rt)^{s/2} = (1+r^2)^{s/2}(1+qt)^{s/2} = (1+r^2)^{s/2}\sum_{n=0}^{\infty} {s/2 \choose n} q^n t^n$$
 (5.61)

According to [FL23, Satz 22.8] the binomial series converges absolutely and uniformly for $-1 \le t \le 1$ and all $0 \le q \le 1$. Hence we can interchange the summation and integration in (5.54) to see that

$$\lambda_{l,s}(r) = (1+r^2)^{s/2} \sum_{n=0}^{\infty} {s/2 \choose n} q^n \frac{1}{2} \int_{-1}^1 t^n P_l(t) dt \quad l \ge 2.$$
 (5.62)

Write

$$t^{n} = \sum_{m=0}^{n} c_{n,m} P_{m}(t) \quad \text{for } t \in [-1, 1].$$
 (5.63)

Using that the Legendre polynomials are orthogonal in $L^2([-1,1])$ and normalized by

$$\frac{1}{2} \int_{-1}^{1} P_l(t)^2 dt = \frac{1}{2l+1},$$

and P_l has degree l, one sees that $\int_{-1}^1 t^n P_l(t) dt = 0$ if n < l and for $n \ge l$ we have $\frac{1}{2} \int_{-1}^1 t^n P_l(t) dt = \frac{c_{n,l}}{1l+1}$. Thus

$$\lambda_{l,s}(r) = (1+r^2)^{s/2} \sum_{n=l}^{\infty} {s/2 \choose n} \frac{q^n c_{n,l}}{2l+1}, \quad l \ge 2.$$
 (5.64)

We will use that the coefficients $c_{n,l}$ for $n, l \in \mathbb{N}_0$ are non-negative, see (A.8) in Appendix A. Moreover,

$$\sum_{m=0}^{n} c_{n,m} = 1,$$

which follows from setting t=1 in (5.63) and using $P_l(1)=1$ for $l\in\mathbb{N}_0$. Together with $c_{n,m}\geq 0$, this also shows $c_{n,m}\leq 1$. From [FL23, Hilfssatz 22.8a] we have the bound

$$\left| \binom{s/2}{n} \right| \le \frac{c}{n^{1+s/2}} \,. \tag{5.65}$$

This implies that the series in the right-hand-side of (5.64) converges absolutely for all $0 \le q \le 1$, since $0 \le c_{n,l} \le 1$ and hence

$$\sum_{n=l}^{\infty} \left| \binom{s/2}{n} \right| \frac{q^n c_{n,l}}{2l+1} \lesssim \sum_{n=l}^{\infty} \frac{1}{2l+1} \frac{1}{n^{1+s/2}} < \infty$$
 (5.66)

for any s > 0. Moreover, we also have

$$\sum_{l\geq 2} \left| \lambda_{l,s}(r) \right| \leq (1+r^2)^{s/2} \sum_{l=2}^{\infty} \sum_{n=l}^{\infty} \left| \binom{s/2}{n} \right| \frac{q^n c_{n,l}}{2l+1} \lesssim \sum_{l=2}^{\infty} \sum_{n=l}^{\infty} \frac{1}{n^{1+s/2}} \frac{1}{2l+1} \\
= \sum_{n=2}^{\infty} \sum_{l=2}^{n} \frac{1}{n^{1+s/2}} \frac{1}{2l+1} \lesssim \sum_{n=2}^{\infty} \frac{\ln(2+n)}{n^{1+s/2}} < \infty .$$
(5.67)

For $n \in \mathbb{N}$ define

$$A_n := \left| \binom{s/2}{n} \right| \sum_{l=2}^n \frac{c_{n,l}}{2l+1}.$$

We have

$$\sum_{l=2}^{\infty} \left| \lambda_{l,s}(r) \right| \le (1 + r^2)^{s/2} \sum_{l=2}^{\infty} \sum_{n=l}^{\infty} \left| \binom{s/2}{n} \right| \frac{c_{n,l}}{2l+1} q^n = (1 + r^2)^{s/2} \sum_{n=2}^{\infty} A_n q^n.$$
 (5.68)

Since $q = 2r/(1 + r^2)$ (see (5.60)) we get

$$\sum_{n=2}^{\infty} A_n q^n \le \frac{4r^2}{(1+r^2)^2} A_2 + \frac{8r^3}{(1+r^2)^3} A_3 + \frac{16r^4}{(1+r^2)^4} \sum_{n=4}^{\infty} A_n . \tag{5.69}$$

In Lemma A.5 in Appendix A we show that

$$A_2 = \left| \binom{s/2}{2} \right| \frac{2}{15}, \quad A_3 = \left| \binom{s/2}{3} \right| \frac{2}{35}, \quad \sum_{k=4}^{\infty} A_k \le \frac{s}{2} \left(\frac{s}{2} - 1 \right) \left(2 - \frac{s}{2} \right) \frac{28}{625}.$$

It follows that

$$\sum_{k=2}^{\infty} A_k q^k \le \frac{r^2}{(1+r^2)^2} f(r,s). \tag{5.70}$$

with f defined in (5.51). Combining (5.70) with (5.68) proves for $s \le 4$

$$C_s(r) = \sum_{l=2}^{\infty} \left| \lambda_{l,s}(r) \right| \le (1 + r^2)^{(s-4)/2} r^2 f(r,s) \le r^2 f(r,s) . \tag{5.71}$$

This proves (5.59), which finishes the proof of Lemma 5.9.

Remark 5.11. We truncate the series in (5.69) at the fourth power because we will later choose $r \lesssim Z^{-1/3}$. As a result, even terms like Zr^4 become negligible as Z increases. For further refinements at small Z respectively large r, it is more appropriate to evaluate the inequality using computational methods.

6. Upper bounds on the weighted kinetic energy

In this section, we derive an upper bound on

$$Z - \frac{1}{2} \frac{\langle |x_1|^s \psi_{N,Z}, P_1^2 \psi_{N,Z} \rangle}{\langle |x_1|^{s-1} \psi_{N,Z}, \psi_{N,Z} \rangle}$$
(6.1)

which is the right-hand side of (3.10). Note that the denominator has to be interpreted in the quadratic form sense

$$\langle |x_1|^s \, \psi_{N,Z}, P_1^2 \psi_{N,Z} \rangle = \langle \nabla_1(|x_1|^s \, \psi_{N,Z}), \nabla_1 \psi_{N,Z} \rangle_{L^2(\mathbb{R}^3 N)}$$

$$= \int_{\mathbb{R}^3(N-1)} \langle |x_1|^s \, \psi_{N,Z}, P_1^2 \psi_{N,Z} \rangle_{L^2(dx_1)} dx_2 \dots dx_N$$

In the case s = 1 Lieb used in [Lie84] the fact that

$$-2\operatorname{Re}\langle |x|\,\varphi, -\Delta\varphi\rangle_{L^2(\mathbb{R}^3)} = \langle \varphi, (|x|\,\Delta + \Delta\,|x|)\varphi\rangle_{L^2(\mathbb{R}^3)} \le 0. \tag{6.2}$$

Thus the second term in (6.1) can be dropped when s=1. Together with $\alpha_{N,1} \geq 1/2$ this recovers Lieb's bound $N_c < 2Z+1$. In [CS13] Chen and Siedentop showed that in dimension d=3 for any $b \in [0,1]$

$$\langle \varphi, (|x|^b \Delta + \Delta |x|^b) \varphi \rangle \le 0$$
 (6.3)

for any $\varphi \in L^2(\mathbb{R}^3)$. For b > 1 (6.3) does not hold in general. Before we proceed let us clarify in what sense we understand the inner product in (6.1). Recall that $\psi_{N,Z} \in \mathcal{H}_N^f$ is the normalized many particle ground-state of $H_{N,Z}$ in (2.1) and does depend on the positions of particles (x_1, x_2, \ldots, x_n) and the spin degrees of freedom $(\sigma_1, \sigma_2, \ldots, \sigma_N)$ with $\sigma_i \in \{1/2, -1/2\}$. Following [LSo₉, Chapter 3] we define the one-particle density by

$$\rho_{\psi_{N,Z}}(x) \coloneqq \sum_{i=1}^{N} \rho_{\psi_{N,Z}}^{i}(x)$$

where

$$\rho^{i}_{\psi_{N,Z}}(x) \coloneqq \int_{\mathbb{R}^{3(N-1)}} |\psi(x_1, \dots x_{i-1}, x, x_{i+1}, \dots x_N)|^2 dx_1 \dots dx_i \dots dx_N.$$

where $d\hat{x}_i$ means that the integration of x_i is omitted. Remember that we ignore any degrees of freedom related to spin. Due to (2.3) we have $\rho^i = \rho^1$ for any $i \in \{1, 2, ..., N\}$ and thus

$$\rho_{\psi_{N,Z}}(x_1) := N\rho_{\psi_{N,Z}}^1(x_1) \tag{6.4}$$

with

$$\int_{\mathbb{R}^3} \rho_{\psi_{N,Z}}(x_1) dx_1 = N.$$

Consequently for any $p \in \mathbb{R}$

$$\langle |x_1|^p \psi_{N,Z}, \psi_{N,Z} \rangle = \frac{1}{N} \int_{\mathbb{R}^3} |x_1|^p \rho_{\psi_{N,Z}}(x_1) dx_1$$
 (6.5)

As a substitute for (6.2) we prove

Lemma 6.1. For any $s \ge 2$

$$\frac{-1}{2} \frac{\left\langle |x_1|^s \psi_{N,Z}, P_1^2 \psi_{N,Z} \right\rangle}{\left\langle |x_1|^{s-1} \psi_{N,Z}, \psi_{N,Z} \right\rangle} \le \frac{s^2 - 1}{8} \left\langle |x_1|^{s-1} \psi_{N,Z}, \psi_{N,Z} \right\rangle^{\frac{-1}{s-1}} . \tag{6.6}$$

Proof. For readability we drop the indices N, Z and write $\psi = \psi_{N,Z}$. Applying the IMS-localization formula, see for example [CFKS87, Theorem 3.2], yields

$$\operatorname{Re}\langle |x_{1}|^{s} \psi, P_{1}^{2} \psi \rangle_{L^{2}(dx_{1})} = \left\langle |x_{1}|^{s/2} \psi, \left[P_{1}^{2} - \left| \frac{\nabla_{1} |x_{1}|^{s}}{2 |x_{1}|} \right|^{2} \right] |x_{1}|^{s/2} \psi \right\rangle_{L^{2}(dx_{1})}$$

$$= \left\langle |x_{1}|^{s/2} \psi, \left[P_{1}^{2} - \frac{s^{2}}{4} |x_{1}|^{-2} \right] |x_{1}|^{s/2} \psi \right\rangle_{L^{2}(dx_{1})}$$

$$\geq \frac{1 - s^{2}}{4} \left\langle |x_{1}|^{s-2} \psi, \psi \right\rangle_{L^{2}(dx_{1})}$$

$$(6.7)$$

Due to (6.5) we have

$$\langle |x_1|^{s-2} \psi, \psi \rangle = \frac{1}{N} \int_{\mathbb{R}^3} |x_1|^{s-2} \rho_{\psi}(x_1) dx_1.$$

Applying Hölder's inequality for

$$p = \frac{s-1}{s-2}, q = s-1$$

yields

$$\left\langle |x_1|^{s-2} \, \psi, \psi \right\rangle_{L^2(dx_1)} \leq \left(\frac{1}{N} \int_{\mathbb{R}^3} |x_1|^{s-1} \, \rho_{\psi}(x_1) \, dx_1 \right)^{\frac{s-2}{s-1}} = \left(\left\langle |x_1|^{s-1} \, \psi, \psi \right\rangle_{L^2(dx_1)} \right)^{\frac{s-2}{s-1}} \, .$$

Note that we used s > 2 in this step. If one wants to cover the cases $s \in (1, 2)$ one needs to estimate the expression above differently. Consequently

$$\frac{\left\langle |x_1|^{s-2} \psi, \psi \right\rangle_{L^2(dx_1)}}{\left\langle |x_1|^{s-1} \psi, \psi \right\rangle_{L^2(dx_1)}} \le \left(\left\langle |x_1|^{s-1} \psi, \psi \right\rangle_{L^2(dx_1)} \right)^{\frac{-1}{s-1}}. \tag{6.8}$$

Combining (6.7) and (6.8) proves Lemma (6.1). The case s = 2 follows in the limit $s \to 2$.

Remark 6.2. There exists a straightforward simplification of the inequality in Lemma 6.1 since by Jensen's Inequality

$$\langle |x_1|^{s-1} \psi_{N,Z}, \psi_{N,Z} \rangle^{\frac{-1}{s-1}} \le \langle |x_1|^{-1} \psi_{N,Z}, \psi_{N,Z} \rangle$$
 (6.9)

The right–hand side of (6.6) is growing quadratic in s which is unfortunate since the bound on b(s) in Theorem 2.2 is decreasing. Note that the right–hand side of (6.9) can be interpreted as the inverse expectation of the radius of the atom which in Thomas–Fermi Theory grows as $Z^{-1/3}$ (see [Lie76, p. 560]) but should be bounded in Z for real atoms. In [Nam12] Nam did control the right–hand side of (6.9). We proceed similarly to his proof.

We continue by estimating the right-hand side of (6.6). We want to apply the following inequality introduced by Lieb in [Lie76, p. 563]

$$\left(\int_{\mathbb{R}^3} f(x)^{\frac{5}{3}} dx\right)^{\frac{p}{2}} \int_{\mathbb{R}^3} |x|^p f(x) dx \ge C_p \left(\int_{\mathbb{R}^3} f(x) dx\right)^{1 + \frac{5p}{6}}$$
(6.10)

which holds for any non negative measurable function f and $p \ge 0$ where the sharp constant C_p is attained for

$$f_p(x) := \begin{cases} (1 - |x|^p)^{\frac{3}{2}} & |x| \le 1\\ 0 & \text{elsewise} \end{cases}$$
 (6.11)

We give the explicit constant C_p in the Appendix in equation (A.18). We prove

Lemma 6.3. Let $p \ge 0$ then

$$\left(\frac{1}{N} \int_{\mathbb{R}^3} |x_1|^p \, \rho_{\psi_{N,Z}}(x_1) \, dx_1\right)^{-1/p} \le \kappa C_p^{-1/p} Z N^{-2/3}$$

where $\kappa = \sqrt{5} \left(\frac{2}{9\pi^2} 1.456 \right)^{1/3}$ and C_p the constant in (6.10).

Proof. Applying (6.10) for $f = \rho_{\psi_{N,Z}}$ yields

$$\left(\frac{1}{N}\int_{\mathbb{R}^3}|x_1|^p\,\rho_{\psi_{N,Z}}(x_1)dx_1\right)^{-1/p}\leq C_p^{-1/p}N^{-5/6}\left(\int_{\mathbb{R}^3}\rho_{\psi_{N,Z}}(x_1)^{\frac{5}{3}}dx_1\right)^{\frac{1}{2}}.$$

By the fermionic kinetic energy inequality in [FNVDB18, Theorem 1]

$$\frac{u^{\frac{-2}{3}}}{2}K_3 \int_{\mathbb{R}^3} \rho_{\psi_{N,Z}}(x)^{\frac{5}{3}} dx \le \sum_{i=1}^N \frac{1}{2} \langle \psi_{N,Z}, [-\Delta_i] \psi_{N,Z} \rangle$$
 (6.12)

with $K_3 = \frac{3}{5} \left(\frac{1.456}{6\pi^2}\right)^{-2/3} \approx 7.096$. Here u denotes the degrees of freedom in the spin components. We consider spin 1/2 particles (for example electrons) and thus u = 2. By the quantum mechanic virial theorem (see [Wei67], [ALHK23])

$$-E_{N,Z} = \sum_{i=1}^{N} \frac{1}{2} \langle \psi_{N,Z}, [-\Delta_i] \psi_{N,Z} \rangle.$$
 (6.13)

Combining (6.12) and (6.13) for u = 2 we arrive at

$$\int_{\mathbb{R}^3} \rho_{\psi_{N,Z}}(x)^{\frac{5}{3}} dx_1 \le -\frac{2^{5/3}}{K_3} E_{N,Z} \,.$$

Together with

$$-E_{N,Z} \le AZ^2 N^{1/3}$$

for $A = (3/2)^{1/3}$ (see Lemma A.7) this yields

$$\left(\frac{1}{N} \int_{\mathbb{R}^3} |x_1|^p \, \rho_{\psi_{N,Z}}(x_1) dx_1\right)^{-1/p} \le C_p^{-1/p} \left(\frac{2^{5/3}}{K_3} A\right)^{1/2} Z N^{-2/3}$$

$$= C_p^{-1/p} \sqrt{5} \left(\frac{2}{9\pi^2} 1.456\right)^{1/3} Z N^{-2/3} .$$

Combining Lemma 6.6 and Lemma 6.3 we can prove

Lemma 6.4. Let $s \ge 2$ then

$$Z + \frac{1}{2} \frac{\left\langle |x_1|^s \psi_{N,Z}, \Delta_1 \psi_{N,Z} \right\rangle}{\left\langle |x_1|^{s-1} \psi_{N,Z}, \psi_{N,Z} \right\rangle} \le Z + \frac{s^2 - 1}{8} C_{s-1}^{-1/(s-1)} \kappa Z N^{-2/3}$$
(6.14)

with $\kappa = \sqrt{5} \left(\frac{2}{9\pi^2} 1.456 \right)^{1/3}$ and C_{s-1} the constant in (6.10).

Proof. The inequality (6.14) follows directly by combining Lemma 6.1 and Lemma 6.3. The fact that we can either apply Lemma 6.3 for p = 1 or p = s - 1 is due to Jensen's inequality as explained in Remark 6.2. An explicit calculation shows

$$C_1^{-1} = \left(3^{\frac{5}{3}} 5^{\frac{5}{6}} \frac{\left(\frac{7}{\pi}\right)^{\frac{1}{3}}}{22\sqrt{11}}\right)^{-1} \approx 2.341 \dots$$

$$C_2^{-1/2} = 4 \frac{\pi^{2/3}}{\sqrt{15}} \approx 2.215 \dots$$

and $p \mapsto C_p^{-1/p}$ is decreasing. We give in Appendix Lemma A.6 the explicit constant C_p for any $p \in [1, 2]$.

7. Bounds on maximal excess charge

From Lemma 5.9 and Lemma 6.4 it is straightforward to prove the inequality in Theorem 2.2. We begin with the general inequality for $s \in [2, 3]$ before we discuss some refinements in the cases s = 2 and s = 3.

7.1. Proof of the Main Theorem.

Proof of Theorem 2.2. We aim to solve (5.50) namely

$$\frac{(1+r)^{s+1} - (1-r)^{s+1}}{2r(s+1)} N\beta_s \le \frac{(1+r)^{s+2} - (1-r)^{s+2}}{2r(s+2)} \left(\alpha_{N,s}(N-1) + \frac{1}{r}\right) + r^2 f(r,s)\alpha_{N,s}(N-1)$$
(7.1)

for N. Note that the fraction on the left–hand side of (7.1) is positive for all r > 0 and s > 0 and consequently we can use the lower bound $b(s)^{-1}$ from Proposition 4.5 to bound the left–hand side β_s .

Direct computations show for $r \in [0, 1]$ and $p \ge 2$

$$2rp \le (1+r)^p - (1-r)^p.$$

Consequently

$$\frac{2r(s+2)}{(r+1)^{s+2} - (1-r)^{s+2}} \le 1$$

together with f(r, s) < 1/2

$$\frac{2r(s+2)}{(r+1)^{s+2}-(1-r)^{s+2}}r^2f(r,s) \le r^2f(r,s) \le \frac{r^2}{2}.$$

Consequently from 5.9 we conclude

$$\left(\frac{s+2}{s+1}\frac{(r+1)^{s+1}-(1-r)^{s+1}}{(r+1)^{s+2}-(1-r)^{s+2}}\frac{N}{b(s)}-\frac{1}{r}\right) \le \alpha_{N,s}(N-1)\left(1+\frac{r^2}{2}\right) \tag{7.2}$$

We prove in the appendix as Lemma A.8 that for any $r \in (0, 1)$ and $s \ge 0$

$$\frac{s+2}{s+1} \frac{(r+1)^{s+1} - (1-r)^{s+1}}{(r+1)^{s+2} - (1-r)^{s+2}} \ge 1 - \frac{s}{3}r^2.$$
 (7.3)

Combining the (7.2) and (7.3) we conclude

$$\left(1 - \frac{s}{3}r^2\right) \frac{N}{b(s)} - \frac{1}{r} < \alpha_{N,s}(N-1) \left(1 + \frac{r^2}{2}\right) \tag{7.4}$$

We minimize the left-hand side of (7.4) and therefore we choose

$$r = \left(\frac{3}{2s}\right)^{1/3} \left(\frac{N}{b(s)}\right)^{-1/3} =: \lambda N^{-1/3}. \tag{7.5}$$

Combining (7.4) and (7.5) to find

$$\frac{N}{b(s)} \le \alpha_{N,s}(N-1) \left(1 + \frac{\lambda^2}{2} N^{-2/3} \right) + \left(\lambda^{-1} + \frac{s}{3} \frac{\lambda^2}{b(s)} \right) N^{1/3}.$$

Applying Lemma 6.14 shows

$$\frac{N}{b(s)} \le Z \left(1 + AN^{-2/3} \right) \left(1 + (\lambda^2/2)N^{-2/3} \right) + \left(\lambda^{-1} + \frac{s}{3} \frac{\lambda^2}{b(s)} \right) N^{1/3}
= Z + \left(A + (\lambda^2/2) \right) ZN^{-2/3} + \left(\lambda^{-1} + \frac{s}{3} \frac{\lambda^2}{b(s)} \right) N^{1/3} + \frac{\lambda^2 A}{2} ZN^{-4/3}$$

where

$$A := \frac{s^2 - 1}{8} C_{s-1}^{-1/(s-1)} \kappa$$

is the parameter in Lemma 6.14. Note that $Z \le N \le 3Z$ and thus there exists some c(s) > 0 such that

$$N_c < b(s) Z + c(s) Z^{1/3}$$

Since the calculations hold for any lower bound $b(s)^{-1} < \beta_s$ the statement of Theorem 2.2 follows.

7.2. The Case of a Quadratic Weight.

Proof of Proposition 2.4. Applying Lemma 5.9 yields

$$\frac{r^2/3+1}{r^2+1}N\beta_2 - \frac{1}{r} \le \alpha_{N,2}(N-1) < Z + \frac{3}{8}C_1^{-1}\kappa ZN^{-2/3}$$
(7.6)

Note that by a straightforward calculation

$$N\beta_2 \left(1 - \frac{2r^2}{3} \right) \le \frac{r^2/3 + 1}{r^2 + 1} N\beta_2 \tag{7.7}$$

and consequently by inserting (7.7) into (7.6) we arrive at

$$N\beta_2 \left(1 - \frac{2r^2}{3} \right) - \frac{1}{r} \le Z + \frac{3}{8} C_1^{-1} \kappa Z N^{-2/3}$$
 (7.8)

Optimizing the left-hand side of (7.8) in r > 0 gives

$$r = \left(\frac{3}{4}\right)^{1/3} (N\beta_2)^{-1/3} . (7.9)$$

Note that r < 1 for N > 1. Inserting (7.9) into (7.8) yields

$$N\beta_2 - \left(\frac{9}{2}\right)^{1/3} (N\beta_2)^{1/3} \le Z + \frac{3}{8}C_1^{-1}\kappa Z N^{-2/3}$$
.

Applying Lemma 6.4 we arrive at

$$N\beta_2 \le Z + \frac{3}{8}C_1^{-1}\kappa ZN^{-2/3} + \left(\frac{9}{2}\beta_2\right)^{1/3}N^{1/3}$$
.

We define

$$\lambda := \frac{3}{8}C_1^{-1}\kappa \approx 0.6284$$
.

Then

$$N\beta_2 \le Z + \lambda Z N^{-2/3} + \left(\frac{9}{2}\beta_2\right)^{1/3} N^{1/3}$$
 (7.10)

Let a > 0 and assume that

$$N\beta_2 \ge Z + \beta_2 a Z^{1/3} \,. \tag{7.11}$$

Combining (7.10) and (7.11) yields

$$Z + \beta_2 a Z^{1/3} \le Z + \lambda Z N^{-2/3} + \left(\frac{9}{2}\beta_2\right)^{1/3} N^{1/3}. \tag{7.12}$$

Dividing by $Z^{1/3}$ gives

$$a \leq \beta_2^{-1} \lambda \left(\frac{N}{Z}\right)^{-2/3} + \beta_2^{-1} \left(\frac{9}{2}\beta_2\right)^{1/3} \left(\frac{N}{Z}\right)^{1/3} \; .$$

From Lieb's bound, we conclude N/Z < 5/2 for any $Z \ge 2$. Maximizing the right hand side of (7.12) for $N/Z \in [1, 5/2]$ yields

$$a \leq \beta_2^{-1} \lambda \left(\frac{N}{Z}\right)^{-2/3} + \beta_2^{-1} \left(\frac{9}{2}\beta_2\right)^{1/3} \left(\frac{N}{Z}\right)^{1/3} \leq 2.953.$$

Thus for a := 2.96 assumption (7.11) cannot hold and thus

$$N \le \frac{1}{\beta_2} Z + 2.96 Z^{1/3} < b(2) Z + 2.96 Z^{1/3}$$

for any $Z \ge 2$. The assertion in Proposition 2.4 follows.

7.3. The Case of a Cubic Weight.

Proof of Proposition 2.5. By application of Lemma 5.9 we find

$$\frac{(1+r)^{s+1} - (1-r)^{s+1}}{2r(s+1)} N\beta_s \le \frac{(1+r)^{s+2} - (1-r)^{s+2}}{2r(s+2)} \left(\alpha_{N,s}(N-1) + \frac{1}{r}\right) + r^2 f(r,s)\alpha_{N,s}(N-1) \tag{7.13}$$

or equivalently

$$\left(\frac{s+2}{s+1}\right) \frac{(1+r)^{s+1} - |1-r|^{s+1}}{(1+r)^{s+2} - |1-r|^{s+2}} N\beta_s - \frac{1}{r} \le \left(1 + \frac{2r(s+2)r^2f(r,s)}{(1+r)^{s+2} - |1-r|^{s+2}}\right) \alpha_{N,s}(N-1)$$
(7.14)

In Appendix A as Lemma A.8 we show that for any $r \in (0, 1)$ and $s \ge 0$

$$1 - \frac{s}{3}r^2 \le \frac{s+2}{s+1} \frac{(r+1)^{s+1} - (1-r)^{s+1}}{(r+1)^{s+2} - (1-r)^{s+2}}.$$
 (7.15)

Combining (7.15) and (7.14) with s = 3 proves

$$(1-r^2)N\beta_3 - \frac{1}{r} \le \left(1 + \frac{5}{r^2(r^2+10)+5}r^2f(r,3)\right)\alpha_{N,3}(N-1). \tag{7.16}$$

where

$$f(r,3) = \frac{1}{5} + \frac{1}{35}r + \frac{168}{625}r^2.$$
 (7.17)

By direct computations one shows for any $r \ge 0$

$$\frac{5}{r^2(r^2+10)+5} \le 1 - 2r^2 + \frac{19}{5}r^4. \tag{7.18}$$

Assume r < 0.5 then by combining (7.17) and (7.18) we find

$$\left(1 + \frac{5}{r^2(r^2 + 10) + 5}r^2 f(r, 3)\right) \le 1 + \frac{r^2}{5} + \frac{r^3}{35} \underbrace{-\frac{82r^4}{625} - \frac{2r^5}{35} + \frac{139r^6}{625} + \frac{19r^7}{175} + \frac{3192r^8}{3125}}_{\le 0, \text{ for } r < 0.53}$$

$$\le 1 + \frac{r^2}{5} + \frac{r^3}{35}.$$
(7.19)

Inserting (7.19) into the right-hand side of (7.16) we arrive at

$$(1 - r^2)N\beta_3 - \frac{1}{r} \le \left(1 + \frac{r^2}{5} + \frac{r^3}{35}\right)\alpha_{N,3}(N - 1). \tag{7.20}$$

for any $r \le 0.5$. Applying Lemma 6.4 for s = 3 yields

$$(1-r^2)N\beta_3 - \frac{1}{r} \le \left(1 + \frac{r^2}{5} + \frac{r^3}{35}\right) \left(Z + cZN^{-2/3}\right), \quad c = C_2^{-1/2}\kappa.$$

We continue by choosing $r \in (0, 0.5]$. As in the previous cases let

$$r = \lambda (N\beta_3)^{-1/3}, \quad \lambda > 0.$$
 (7.21)

Inserting (7.21) into (6.4) yields

$$N\beta_{3} \leq Z + \lambda^{-1}(N\beta_{3})^{1/3} + \lambda^{2}(N\beta_{3})^{1/3} + \frac{\lambda^{2}}{5}(N\beta_{3})^{-2/3}Z + cZN^{-2/3}$$

$$+ \frac{\lambda^{3}}{35}(N\beta_{3})^{-1}Z + c\frac{\lambda^{2}}{5}(N\beta_{3})^{-2/3}ZN^{-2/3}$$

$$+ c\frac{\lambda^{3}}{35}(N\beta_{3})^{-1}ZN^{-2/3}$$

$$(7.22)$$

We can always assume $Z < N\beta_3$ (since otherwise $N \le \beta_3^{-1}Z$ already proves an inequality than the statement) and consequently we find

$$N\beta_{3} \leq Z + \left(\lambda^{-1} + \frac{6\lambda^{2}}{5}\right) (N\beta_{3})^{1/3} + cZN^{-2/3} + \frac{\lambda^{3}}{35} + c\frac{\lambda^{2}}{5} (\beta_{3})^{1/3} N^{-1/3} + c\frac{\lambda^{3}}{35} N^{-2/3}$$

$$(7.23)$$

To optimize the leading correction term that grows as $N^{1/3}$ we minimize

$$\lambda \mapsto \lambda^{-1} + \frac{6}{5}\lambda^2$$
,

and consequently, we choose

$$\lambda = \left(\frac{5}{12}\right)^{1/3}$$
, such that $\lambda^{-1} + \frac{6}{5}\lambda^2 = 3\left(\frac{3}{10}\right)^{1/3}$. (7.24)

To ensure r < 0.5 as assumed after (7.24) we need to have

$$N > \frac{10}{3\beta_3} > \frac{10}{3} \,. \tag{7.25}$$

We always assume $N \ge Z$ and consequently the result will hold for $Z \ge 4$. Inserting (7.24) into (7.23) yields

$$N\beta_{3} \leq Z + 3\left(\frac{3}{10}\right)^{1/3} (N\beta_{3})^{1/3} + cZN^{-2/3} + \frac{1}{84} + \frac{c}{5}\left(\frac{5}{12}\right)^{2/3} (\beta_{3})^{1/3}N^{-1/3} + c\frac{1}{84}N^{-2/3}$$

$$(7.26)$$

We can always assume $N \ge \beta_3^{-1}Z$ because otherwise $N \le \beta_3^{-1}Z$ and we are done. Inserting $N \ge \beta_3^{-1}Z$ into the last two summands in the right-hand side of (7.26) yields

$$N\beta_3 \le Z + 3\left(\frac{3}{10}\right)^{1/3} (N\beta_3)^{1/3} + cZN^{-2/3} + \frac{1}{84} + \frac{c}{5}\left(\frac{5}{12}\right)^{2/3} (\beta_3)^{2/3}Z^{-1/3} + c\frac{\beta_3^{2/3}}{84}Z^{-2/3}.$$

To prove the desired inequality

$$N \le \beta_3^{-1} Z + a_1 Z^{1/3} + a_2 + a_3 Z^{-1/3} + a_4 Z^{-2/3}.$$

for optimal $a_1, a_2, a_3, a_4 \ge 0$ and all $N \ge 3$ we assume that for any arbitrary but fixed N, Z with $N \ge 3$ holds

$$N\beta_3 \ge Z + \beta_3 a_1 Z^{1/3} + \beta_3 a_2 + \beta_3 a_3 Z^{-1/3} + \beta_3 a_4 Z^{-2/3}$$
(7.27)

and bring this to a contradiction by choosing a_1 , a_2 , a_3 , $a_4 \ge 0$ and comparing (7.27) with (7.26). We do this now to finish the proof. Combining (7.27) with (7.26) yields

$$\beta_{3}a_{1}Z^{1/3} + \beta_{3}a_{2} + \beta_{3}a_{3}Z^{-1/3} + \beta_{3}a_{4}Z^{-2/3}$$

$$\leq 3\left(\frac{3}{10}\right)^{1/3} (N\beta_{3})^{1/3} + cZN^{-2/3} + \frac{1}{84}$$

$$+ \frac{c}{5}\left(\frac{5}{12}\right)^{2/3} (\beta_{3})^{2/3}Z^{-1/3} + c\frac{\beta_{3}^{2/3}}{84}Z^{-2/3}$$
(7.28)

After comparing both sides of (7.28) we choose

$$a_2 = \beta_3^{-1}/84$$
, $a_3 = \frac{c}{5} \left(\frac{5}{12}\right)^{2/3} \beta_3^{-1/3}$, $a_4 = c \frac{\beta_3^{-1/3}}{84}$. (7.29)

Using β_3^{-1} < 1.1185 and c < 1.5855 this gives

$$a_2 \le 0.0134, \quad a_3 \le 0.184, \quad a_4 \le 0.0196.$$
 (7.30)

For this choice of a_2 , a_3 , a_4 we arrive at

$$\beta_3 a_1 Z^{1/3} \le 3 \left(\frac{3}{10}\right)^{1/3} (N\beta_3)^{1/3} + cZN^{-2/3}$$
 (7.31)

Dividing (7.31) by $\beta_3 Z^{1/3}$ we find

$$a_1 \le 3 \left(\frac{3}{10}\right)^{1/3} \beta_3^{-2/3} \left(\frac{N}{Z}\right)^{1/3} + c\beta_3^{-1} \left(\frac{N}{Z}\right)^{-2/3}$$
 (7.32)

We can always assume $N \ge \beta_3^{-1}Z$ as explained earlier and N < 2Z + 1 due to Lieb's result and consequently we can assume $N/Z \in [\beta_3^{-1}, 5/2]$ for $Z \ge 2$. Thus

$$a_1 \le \sup \left\{ 3 \left(\frac{3}{10} \right)^{1/3} \beta_3^{-2/3} x^{1/3} + c \beta_3^{-1} x^{-2/3} : x \in [\beta_3^{-1}, 5/2] \right\}$$
 (7.33)

Following Lemma 6.4 we have

$$c = \sqrt{5} \left(\frac{2}{9\pi^2} 1.456 \right)^{1/3} 4 \frac{\pi^{2/3}}{\sqrt{15}},\tag{7.34}$$

and since $\beta_3^{-1} \in [1.0, 1.1185]$ one can show that the supremum in the right-hand side of (7.33) is attained at $x = \beta_3^{-1}$ and consequently

$$a_1 \le 3 \left(\frac{3}{10}\right)^{1/3} \beta_3^{-1} + c\beta_3^{-1/3} < 3.893.$$
 (7.35)

For the choice $a_1 = 3.90$ and a_2 , a_3 , a_4 as in (7.28) the inequality (7.27) fails and therefore we find

$$N \leq \beta_3^{-1} Z + 3.90 Z^{1/3} + 0.0134 + 0.184 Z^{-1/3} + 0.0196 Z^{-2/3}, \quad Z \geq 4 \,.$$

this proves the statement of of Proposition 2.5.

APPENDIX A. TECHNICAL DETAILS

A.1. Density Argument for $\alpha_{N,s}$.

Lemma A.1. Let $\alpha_{N,s}$ be defined as in equation (5.1) and $A \subset \mathbb{R}^{3N}$ be defined as

$$A_0 = \{(x_1, x_2, \dots x_N) \in A : x_k \neq 0 \text{ for } 1 \leq k \leq N\}$$

then

$$\alpha_{N,s} = \inf \left\{ \frac{\sum_{1 \le i,k \le N} \frac{|x_k|^s + |x_i|^s}{|x_i - x_k|}}{2(N-1) \sum_{k=1}^N |x_k|^{s-1}} : (x_1, x_2, \dots x_N) \in A_0 \right\}$$
(A.1)

Proof. We define

$$F(x_1, x_2, ..., x_N) := \frac{\sum_{1 \le i, k \le N} \frac{|x_k|^s + |x_i|^s}{|x_i - x_k|}}{2(N-1) \sum_{k=1}^N |x_k|^{s-1}}$$
(A.2)

Note that F is continuous in A and A_0 is dense in A. Since any $(x_1, x_2, ..., x_N) \in A$ consists of arbitrary but distinct point in \mathbb{R}^3 we may always assume that $|x_1| \leq |x_2| \leq \cdots \leq |x_N|$ by relabeling the indices. Since the vectors are distinct only x_1 may vanish. The set A_0 is a subset of A and thus

$$\alpha_{N,s} \leq \inf\{F(x_1, x_2, \dots, x_N) : (x_1, x_2, \dots, x_N) \in A_0\} =: \zeta_{N,s}$$

The claim follows if we can show $\zeta_{N,s} \leq \alpha_{N,s}$. We show for arbitrary $\varepsilon > 0$ that $\zeta_{N,s} \leq \alpha_{N,s} + \varepsilon$ and conclude the statement in the limit $\varepsilon \to 0$. Let $\varepsilon > 0$ arbitrary then by the definition of the infimum, there exists some $r_{\varepsilon} \in A$ such that $F(r_{\varepsilon}) \leq \alpha_{N,s} + \varepsilon/2$. If $r_{\varepsilon} \in A_0$ then $F(r_{\varepsilon}) \geq \zeta_{N,s}$ and the inequality follows directly. If $r_{\varepsilon} \in A \setminus A_0$ then $(r_{\varepsilon})_1 = 0$. By continuity of F in r_{ε} we can find $u_{\varepsilon} \in A_0$ such that $|F(r_{\varepsilon}) - F(u_{\varepsilon})| \leq \varepsilon/2$ and thus

$$\zeta_{N,s} \leq F(u_{\varepsilon}) \leq \alpha_{N,s} + \varepsilon.$$

Thus we have shown $\zeta_{N,s} = \alpha_{N,s}$ and the statement follows immediately.

A.2. Funk-Hecke formula and Multipol Moments.

Lemma A.2. For any function $f \in L^1(-1,1)$ and any Legendre polynomial P_l we have

$$\frac{1}{4\pi} \int_{S^2} f(\xi \cdot \omega) P_l(\zeta \cdot \omega) d\omega = \lambda P_l(\xi \cdot \zeta) \tag{A.3}$$

for all $\xi, \zeta \in S^2$ where

$$\lambda = \frac{1}{2} \int_{-1}^{1} P_l(t) f(t) dt$$

Proof. This is a direct consequence of the Funk–Hecke formula in three dimensions, see equation (2.66) just after Theorem 2.22 in Chapter 2.6 of [AH12].

Lemma A.3. Let $\lambda > -2, a \in \mathbb{R}^3$ and r, |a| > 0, then

$$\int_{S^2} |a + r\omega|^{\lambda} \frac{d\omega}{4\pi} = \frac{(|a| + r)^{\lambda + 2} - (|a| - r)^{\lambda + 2}}{2r |a| (\lambda + 2)}$$

Proof. Since the Legendre polynomial $P_0 = 1$ and $|a + r\omega|^2 = |a|^2 + r^2 + 2r|a|\widehat{a} \cdot \omega$ we see from Lemma A.2 that

$$\int_{S^2} |a + r\omega|^t \, \lambda \frac{d\omega}{4\pi} = \frac{1}{2} \int_{-1}^1 (|a|^2 + r\omega + 2r \, |a| \, t)^{\lambda/2} \frac{d\omega}{4\pi} = \frac{(|a| + r)^{\lambda+2} - (|a| - r)^{\lambda+2}}{2r \, |a| \, (\lambda + 2)}$$

Lemma A.4. Let $s \ge -2$, $\zeta \in S^2$, $w \in \mathbb{R}^3 \setminus \{0\}$, and r > 0. Then

$$\begin{split} & \int_{S^2} |w + r\omega|^s \frac{d\omega}{4\pi} = \frac{(|w| + r)^{s+2} - ||w| \, 1 - r|^{s+2}}{2r \, |w| \, (s+2)} \\ & \int_{S^2} |w + r\omega|^s \, \langle \zeta, \omega \rangle \frac{d\omega}{4\pi} = c(|r|) \langle w, \zeta \rangle \\ & \int_{S^2} |w + r\omega|^s \, P_l(\langle \hat{w}, \omega \rangle) \frac{d\omega}{4\pi} = \frac{1}{2} \int_{-1}^1 (w^2 + r^2 + 2r \, |w| \, t)^{s/2} P_l(t) dt \end{split}$$

where $c(r) := \int_{-1}^{1} (1 + r^2 + 2rt)^{s/2} t \, dt$ and $c_{k,n} := (2n + 1) \int_{-1}^{1} t^k P_n(t) \, dt$.

Proof. The zero-order moment is easy to and follows directly from Lemma A.3. Similar

$$\int_{S^2} |\hat{x}_j + r\omega|^s P_1(\langle \hat{a}, \omega \rangle) \frac{d\omega}{4\pi} = \int_{S^2} |\hat{x}_j + r\omega|^s \langle \hat{a}, \omega \rangle \frac{d\omega}{4\pi}$$

$$= \langle \hat{a}, \int_{S^2} |\hat{x}_j + r\omega|^s \omega \frac{d\omega}{4\pi} \rangle$$

$$= \langle U^{-1} \hat{a}, \int_{S^2} |U^{-1} \hat{x}_j + r\omega|^s \omega \frac{d\omega}{4\pi} \rangle$$

for any $U \in SO(3)$. Choose $U \in SO(3)$ such that $U^{-1}\hat{x}_j = \hat{e}_3$ then

$$\int_{S^2} \left| U^{-1} \hat{x}_j + r\omega \right|^s \omega \frac{d\omega}{4\pi} = \int_{S^2} |\hat{e}_3 + r\omega|^s \omega \frac{d\omega}{4\pi}$$

$$= 2\pi \hat{e}_3 \int_0^{\pi} (1 + r^2 + 2r\cos\theta)^{s/2} \cos\theta \frac{\sin\theta d\theta}{4\pi}$$

$$= \frac{\hat{e}_3}{2} \int_{-1}^{1} (1 + r^2 + 2rt)^{s/2} t dt =: \hat{e}_3 c(r)$$

and thus

$$\int_{S^2} |\hat{x}_j + r\omega|^s P_1(\langle \hat{a}, \omega \rangle) \frac{d\omega}{4\pi} = c(r) \langle \hat{a}, U\hat{e}_3 \rangle$$
(A.4)

for some $c(r) \ge 0$. To compute higher multipole moments we need to extend $|\hat{x_j} + r\omega|^s$ in terms of Legendre polynomials. Note, that

$$|\hat{x}_j + r\omega|^s = (1 + r^2 + 2r\langle \hat{x}_j, \omega \rangle)^{s/2} = (1 + r^2)^{s/2} \left(1 + \frac{2r}{1 + r^2}\langle \hat{x}_j, \omega \rangle\right)^{s/2}$$
(A.5)

For convenience we define

$$q \coloneqq \frac{2r}{1+r^2} \, .$$

By Newton's generalized binomial theorem, we can extend the right-hand side of equation (A.5)

$$(1+r^2)^{s/2} \left(1 + \frac{2r}{1+r^2} \langle \hat{x}_j, \omega \rangle \right)^{s/2} = (1+r^2)^{s/2} \sum_{k=0}^{\infty} {s/2 \choose k} q^k \left(\langle \hat{x}_j, \omega \rangle \right)^k \tag{A.6}$$

which converges absolutely since $q(\hat{x}_j, \omega) \leq 1$ by assumption. If $s/2 \in \mathbb{N}$ then the generalized binomial coefficients are identical to the normal binomial coefficients with

$$\binom{s/2}{k} = 0, \quad k > s/2 \in \mathbb{N}$$
 (A.7)

and hence the series above is only a finite sum in that case. If $s/2 \notin \mathbb{N}$ then for any $k \in \mathbb{N}_0$ the generalized binomial coefficients are defined as

$$\binom{s/2}{k} = \frac{\frac{s}{2}(\frac{s}{2}-1)\cdots(\frac{s}{2}-(k-1))}{k!} = \frac{\prod_{n=0}^{k-1}(\frac{s}{2}-n)}{k!}.$$

We extend monomials in terms of Legendre polynomials. From Rodrigou's Formula, one can derive the explicit representation

$$P_n(t) = 2^n \sum_{m=0}^n t^m \binom{n}{m} \binom{\frac{n+m-1}{2}}{n}$$

(See [AS64][Chapter 8]). Let

$$c_{k,n} := \frac{(2n+1)}{2} \int_{-1}^{1} t^{k} P_{n}(t) dt$$

$$= (2n+1)2^{n-1} \sum_{m=0}^{n} \binom{n}{m} \binom{\frac{n+m-1}{2}}{n} \int_{-1}^{1} t^{k+m} dt$$
(A.8)

then its clear that $c_{k,n} = 0$ for n > k. We differ the cases for which k is even and for which k is odd. When k is even then $c_{k,n} = 0$ whenever n is odd as one easily concludes from equation (A.8). Analogous when k is odd $c_{k,n} = 0$ whenever n is even. Hence for $n \le k$,

$$c_{k,n} = \begin{cases} (2n+1)2^{n-1} \sum_{m=0}^{n} \binom{n}{m} \left(\frac{n+m-1}{2}\right) \frac{2}{k+m+1}, & k+m \text{ is even,} \\ 0, & k+m \text{ is odd,} \\ 1, & k=m=0 \end{cases}$$
 (A.9)

By the orthogonality of Legendre Polynomials

$$\int_{-1}^{1} P_n(t) P_m(t) dt = \frac{2\delta_{mn}}{2n+1}$$

it then follows

$$t^{k} = \sum_{l=0}^{k} c_{k,l} P_{l}(t) . {(A.10)}$$

By the usual definition of the double factorial, one can derive by elementary steps that

$$t^{k} = \sum_{l=k,k-2,\dots} \frac{(2l+1)k!}{2^{(k-l)/2} \left(\frac{k-l}{2}\right)! (l+k+1)!!} P_{k}(t). \tag{A.11}$$

For even numbers of k = 2n with $n \in \mathbb{N}_0$ this means

$$t^{2n} = \sum_{u=0}^{n} \frac{(4u+1)(2n)!}{2^{(n-u)}(n-u)!(2(n+u)+1)!!} P_{2u}(t). \tag{A.12}$$

and for odd numbers of k = 2n + 1 with $n \in \mathbb{N}_0$ this is

$$t^{2n+1} = \sum_{u=0}^{n} \frac{(4u+3)(2n+1)!}{2^{(n-u)}(n-u)!(2(n+u)+3)!!} P_{2u+1}(t). \tag{A.13}$$

Combining the equation (A.10), (A.6) and (A.5) shows

$$|\hat{x}_j + r\omega|^s = (1 + r^2)^{s/2} \sum_{k=0}^{\infty} {s/2 \choose k} q^k \sum_{n=0}^k c_{k,n} P_n(\langle \hat{x}_j, \omega \rangle). \tag{A.14}$$

Using this representation we can compute the remaining multipole moments. For $l \geq 2$ we compute

$$\int_{S^2} \left| \hat{x}_j + r\omega \right|^s P_l(\langle \hat{a}, \omega \rangle) \frac{d\omega}{4\pi}
= (1 + r^2)^{s/2} \sum_{k=0}^{\infty} {s/2 \choose k} q^k \sum_{n=0}^k c_{k,n} \int_{S^2} P_n(\langle \hat{x}_j, \omega \rangle) P_l(\langle \hat{a}, \omega \rangle) \frac{d\omega}{4\pi}.$$
(A.15)

The remaining integral follows from the orthogonality of Legendre Polynomials. By extending the Legendre Polynomials P_n into the spherical harmonics Y_{nm} one easily shows the following orthogonality relation for $a, b \in \mathbb{R}^3$ with ||a|| = ||b|| = 1,

$$\int_{S^{2}} P_{l}(\langle \omega, a \rangle) P_{n}(\langle \omega, b \rangle) \frac{d\omega}{|S^{2}|}
= \sum_{m'=-l}^{l} \sum_{m=-n}^{n} \frac{4\pi}{2l+1} \frac{4\pi}{2n+1} \int_{S^{2}} Y_{lm}^{*}(\omega) Y_{nm'}(\omega) \frac{d\omega}{|S^{2}|} Y_{lm}^{*}(a) Y_{nm'}(b)
= \sum_{m'=-l}^{l} \sum_{m=-n}^{n} \frac{4\pi}{2l+1} \frac{4\pi}{2n+1} \frac{\delta_{mm'} \delta_{ln}}{|S^{2}|} Y_{lm}(a) Y_{nm'}^{*}(b)
= \frac{\delta_{ln}}{2l+1} P_{l}(\langle a, b \rangle).$$
(A.16)

Thus combining equation (A.16) and (A.15) shows for $l \ge 2$,

$$\int_{S^2} \left| \hat{x}_j + r\omega \right|^s P_l(\langle \hat{a}, \omega \rangle) \frac{d\omega}{4\pi}$$

$$= (1 + r^2)^{s/2} \sum_{k=2}^{\infty} {s/2 \choose k} q^k \sum_{n=0}^k c_{k,n} \frac{\delta_{ln}}{2l+1} P_l(\langle \hat{a}, \hat{x}_j \rangle)$$

$$= (1 + r^2)^{s/2} \sum_{k=l}^{\infty} {s/2 \choose k} \frac{q^k c_{k,l}}{2l+1} P_l(\langle \hat{a}, \hat{x}_j \rangle)$$
(A.17)

where the series still converges absolutely as mentioned after equation (A.6). Note that in the case s = 2 the expression vanishes due to equation (A.7).

Lemma A.5. For $s \in [2,3], k \in \mathbb{N}$ with $k \geq 2$ let

$$A_k = \left| \binom{s/2}{k} \right| \sum_{l=2}^k \frac{c_{k,l}}{2l+1}$$

with $c_{k,l}$ defined in equation (A.8). Then

$$\sum_{k=4}^{\infty} A_k \le \frac{s}{2} \left(\frac{s}{2} - 1 \right) \left(2 - \frac{s}{2} \right) \frac{28}{625}.$$

Proof. Note that

$$\sum_{l=0}^{k} c_{k,l} = 1$$

due to its defining equation

$$t^k = \sum_{l=0}^k c_{k,l} P_l(t) .$$

by choosing t = 1 and noting $P_l(1) = 1$ for any $l \in \mathbb{N}$. Consequently

$$A_k \le \frac{1}{5} \left| \binom{s/2}{k} \right| \sum_{l=2}^k c_{k,l} \le \frac{1}{5} \left| \binom{s/2}{k} \right| \sum_{l=0}^k c_{k,l} = \frac{1}{5} \left| \binom{s/2}{k} \right|$$

where we used $c_{k,l} \ge 0$ (see their explicit form in (A.8)). For the generalized binomial coefficients the inequality

$$\left| \binom{s/2}{k} \right| \le \frac{\frac{s}{2}(\frac{s}{2} - 1)}{k(k - 1)} \le \frac{s}{2} \left(\frac{s}{2} - 1 \right) \left(\frac{1}{k - 1} - \frac{1}{k} \right)$$

holds for any $s \in [2, 3]$ and $k \ge 2$, $k \in \mathbb{N}$. Thus for $n_0 \in \mathbb{N}$

$$\sum_{k=n_0}^{\infty} A_k \le \sum_{k=n_0}^{N} A_k + \frac{s}{2} \left(\frac{s}{2} - 1 \right) \frac{1}{5(N-1)}$$

and consequently

$$\sum_{k=N}^{\infty} A_k < \frac{s}{2} \left(\frac{s}{2} - 1 \right) \left(2 - \frac{s}{2} \right) \frac{2}{5(N-1)} =: \delta(N)$$

is arbitrary small for N large enough. Thus we can estimate the series over A_k to arbitrary precision. Let $n_0 = 4$ then

$$\sum_{k=n_0}^{\infty} A_k \le \sum_{k=4}^{2} N A_k + \delta(2N) = \sum_{k=2}^{N} A_{2k} + \sum_{k=2}^{N-1} A_{2k+1} + \delta(2N)$$

With the explicit expression of $c_{k,l}$ in (A.12) we find

$$A_{2k} \le \frac{s}{2} \left(\frac{s}{2} - 1 \right) \left(2 - \frac{s}{2} \right) \sum_{l=1}^{k} \frac{(2k-2)!}{2^{k-l} (k-l)! (2(k+l)+1)!!}$$

and analogous with (A.13)

$$A_{2k-1} \le \frac{s}{2} \left(\frac{s}{2} - 1 \right) \left(2 - \frac{s}{2} \right) \sum_{l=1}^{k} \frac{(2k-1)!}{2^{k-l} (k-l)! (2(k+l)+3)!!}$$

Choosing N = 1000 and computing those terms on a computer explicitly we find

$$\sum_{k=4}^{1001} A_k \le \frac{s}{2} \left(\frac{s}{2} - 1 \right) \left(2 - \frac{s}{2} \right) (0.0242 + 0.0203)$$

Adding the error estimate

$$\delta(2000) \le \frac{s}{2} \left(\frac{s}{2} - 1\right) \left(2 - \frac{s}{2}\right) 0.0003$$

such that

$$\sum_{k=4}^{\infty} A_k \le \frac{s}{2} \left(\frac{s}{2} - 1 \right) \left(2 - \frac{s}{2} \right) \frac{448}{10000}$$

A.3. Explicit constant in an inequality due to Lieb.

Lemma A.6. For any $p \in [1, 2]$ the constant C_p in equation (6.10) is given by

$$C_p = \frac{3\sqrt{\pi}}{4} \frac{(4\pi)^{-p/3}}{p^{1+p/2}} \frac{\left(\frac{15\sqrt{\pi}}{8} \frac{\Gamma(3/p)}{\Gamma(7/2+3/p)}\right)^{p/2} \frac{\Gamma(3/p+1)}{\Gamma(3/p+7/2)}}{\left(\frac{\sqrt{\pi}}{4} \frac{\Gamma(3/p+1)}{\Gamma(3/p+5/2)}\right)^{1+5p/6}}$$
(A.18)

where Γ is the Gamma function defined by the improper integral

$$\Gamma(r) := \int_0^\infty x^{r-1} e^{-x} dx.$$

Proof. We give only a sketch of the calculations. Following [Lie76][p. 563] one needs to solve the following three integrals

$$\int_{\mathbb{R}^3} f_p(x) dx, \, \int_{\mathbb{R}^3} |x|^p f_p(x) dx \text{ and } \int_{\mathbb{R}^3} [f_p(x)]^{5/3} dx$$

for

$$f_p(x) := \begin{cases} (1 - |x|^p)^{\frac{3}{2}} & |x| \le 1\\ 0 & \text{elsewise} \end{cases}$$
 (A.19)

the first integral can be solved by a straightforward calculation and the latter two can be solved by substituting $u = |x|^p$. The first integral reduces to

$$\int_0^1 r^2 (1 - r^p)^{3/2} dr = \frac{\sqrt{\pi}}{4} \frac{\Gamma(3/p + 1)}{\Gamma(3/p + 5/2)}.$$

After substituting the second integral reduces to

$$\frac{1}{p} \int_0^1 u^{3/p} (1-u)^{3/2} du = \frac{3\sqrt{\pi}}{4p} \frac{\Gamma(3/p+1)}{\Gamma(3/p+7/2)}.$$

The third integral reduces to

$$\frac{1}{p} \int_0^1 u^{(3-p)/p} (1-u)^{5/2} du = \frac{15\sqrt{\pi}}{8p} \frac{\Gamma(3/p)}{\Gamma(3/p+7/2)}.$$

Combining these three integrals gives the desired constant.

A.4. **Bound on the Groundstate Energie of the Bohr Atom**. The following Lemma is a well-known fact. We include it here for convenience.

Lemma A.7. Given the operator in (2.1) (in atomic units) for N fermions with $u \in \mathbb{N}$ spin-degrees of freedom and nuclear charge Z then the ground state energy is bound by

$$-E_{N,Z} \le AZ^2 N^{1/3}$$

with $A = \frac{1}{2}u^{2/3}3^{1/3}$.

Proof. The energy levels of hydrogen with nuclear charge Z

$$h := -\frac{1}{2}\Delta - \frac{Z}{|x|} \tag{A.20}$$

are

$$E_n = \frac{-Z^2}{n^2} Ry \tag{A.21}$$

where *Ry* is the Rydberg energy. In atomic units

$$Ry = \frac{m_e e^2}{2(4\pi\varepsilon_0)^2\hbar} = \frac{1}{2} \tag{A.22}$$

Each of these energy levels n^2 -times degenerated. Note that the interelectronic repulsion is a positive contribution to the operator in (2.1) and thus

$$H_{N,Z} \ge \sum_{i=1}^{N} \left(-\frac{1}{2} \Delta_i - \frac{Z}{|x_i|} \right) \tag{A.23}$$

The ground state of the right-hand side can be computed explicitly in terms of the energies in equation (A.21). Due to the fermionic symmetry, the particles occupy the energy levels starting from the lowest counting the degeneration in the ground state. Let $E_0(N, Z)$ the ground-state energy of the right hand side of equation (A.23) and Denote by $L \in \mathbb{N}$ the last completely filled energy Level then there exists $c \in [0, 1)$ such that

$$E_0(N,Z) = cu(L+1)^2 E_{L+1} + u \sum_{j=1}^L j^2 E_j = -uZ^2 R_y(c+L).$$

Here we have used that due to the spin of the particles, each state can be u-times occupied. It remains to compare L with N.

$$\frac{N}{u} = c(L+1)^2 + \sum_{i=1}^{L} j^2 = c(L+1)^2 + \frac{L^3}{3} + \frac{L^2}{2} + \frac{L}{6}$$

A straightforward calculation using $c \in [0, 1]$ shows

$$(L+c)^3 \le \frac{3N}{u}$$

We conclude

$$-E_{N,Z} \le -E_0(N,Z) \le uZ^2 R_y \left(\frac{3N}{u}\right)^{1/3} = \frac{1}{2} u^{2/3} 3^{1/3} Z^2 N^{1/3}.$$

A.5. An Useful Inequality.

Lemma A.8. Let $0 < |r| \le 1$ and $p \ge 1$ then

$$\frac{(1+r)^{p-1} - (1-r)^{p-1}}{2r(p+1)} \ge \frac{(1+r)^p - (1-r)^p}{2rp} \\
\ge \left(1 - \frac{p-1}{3}r^2\right) \frac{(1+r)^{p+1} - (1-r)^{p+1}}{2r(p+1)}.$$
(A.24)

Proof. Since the inequalities in (A.24) are symmetric under changing r to -r, it is enough to prove them for $0 < r \le 1$. In this case (A.24) is equivalent to

$$\frac{(1+r)^{p+1} - (1-r)^{p+1}}{p+1} \ge \frac{(1+r)^p - (1-r)^p}{p} \\
\ge \left(1 - \frac{p-1}{3}r^2\right) \frac{(1+r)^{p+1} - (1-r)^{p+1}}{p+1}.$$
(A.25)

The first bound,

$$h(r) := \frac{(1+r)^{p+1} - (1-r)^{p+1}}{(p+1)} \ge \frac{(1+r)^p - (1-r)^p}{p} =: k(r)$$
 (A.26)

for $r \ge 0$ is easy to show. Since h(0) = 0 = k(0) it follows as soon as $h'(r) \ge k'(r)$ for $r \ge 0$. This is equivalent to

$$(1+r)^p + (1-r)^p \ge (1+r)^{p-1} - (1-r)^{p-1}$$
 for $0 \le r \le 1$. (A.27)

Expanding

$$(1+r)^{p} \pm (1-r)^{p} = (1+r)^{p-1}(1+r) \pm (1-r)^{p-1}(1-r)$$

$$= (1+r)^{p-1} \pm (1-r)^{p-1} + r((1+r)^{p-1} \mp (1-r)^{p-1})$$
(A.28)

in the left-hand-side of (A.27) we see that (A.27) is equivalent to

$$r\left((1+r)^{p-1} - (1-r)^{p-1}\right) \ge 0$$

for $0 \le r \le 1$, which is true if $p \ge 1$. This proves the first bound in (A.25).

We prove the second inequality in (A.25) by determining $c \in \mathbb{R}$ such that

$$f_1(r) := \frac{(1+r)^p - (1-r)^p}{p} \ge \left(1 - cr^2\right) \frac{(1+r)^{p+1} - (1-r)^{p+1}}{(p+1)} =: g_1(r), \tag{A.29}$$

for $0 \le r \le 1$. At r = 0 we have $f_1(0) = g_1(0)$, so (A.29) is true for $r \ge 0$ as soon as $f_1'(r) \ge g_1'(r)$ for $0 \le r \le 0$. This is equivalent to

$$(1+r)^{p-1} + (1-r)^{p-1} \ge (1-cr^2) \left((1+r)^p + (1-r)^p \right)$$

$$\frac{2cr \left((1+r)^{p+1} - (1-r)^{p+1} \right)}{p+1}$$
(A.30)

Using (A.28) this ie equivalent to

$$f_2(r) := -\left((1+r)^{p-1} - (1-r)^{p-1}\right) + \frac{2c}{p+1}\left((1+r)^{p+1} - (1-r)^{p+1}\right) + cr\left((1+r)^p + (1-r)^p\right) \ge 0 \quad \text{for } 0 \le r \le 1.$$
(A.31)

Since $f_2(0) = 0$ we know that (A.31) holds as soon as $f_2'(r) \ge 0$ for $0 \le r \le 1$. Now

$$f_2'(r) = -(p-1)\left((1+r)^{p-2} + (1-r)^{p-2}\right) + 3c\left((1+r)^p + (1-r)^p\right) + cpr\left((1+r)^{p-1} - (1-r)^{p-1}\right)$$

and using (A.28) twice, the second time with p replaced with p-1, we have

$$(1+r)^{p} \pm (1-r)^{p} = (1+r)^{p-2} \pm (1-r)^{p-2} + 2r\left((1+r)^{p-2} \mp (1-r)^{p-2}\right) + r^{2}\left((1+r)^{p-2} \pm (1-r)^{p-2}\right).$$

Hence we see that

$$\begin{split} f_2'(r) &= (3c - (p-1)) \left((1-r)^{p-2} + (1+r)^{p-2} \right) \\ &+ (6+p)cr \left((1+r)^{p-2} - (1-r)^{p-2} \right) \\ &+ (3+p)cr^2 \left((1+r)^{p-2} + (1-r)^{p-2} \right) \geq 0 \end{split}$$

for all $0 \le r \le 1$ as soon as $c \ge (p-1)/3 \ge 0$. This proves the second inequality in (A.25) and finishes the proof of (A.24).

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