THE LARGE - Z BEHAVIOUR OF PSEUDO-RELATIVISTIC ATOMS

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ABSTRACT. In this paper we study the large - Z behaviour of the ground state energy of atoms with electrons having relativistic kinetic energy $\sqrt{p^2c^2+m^2c^4}-mc^2$. We prove that to leading order in Z the energy is the same as in the non-relativistic case, given by (non-relativistic) Thomas-Fermi theory. For the problem to make sense, we keep the product $Z\alpha$ fixed (here α is Sommerfeld's fine structure constant), and smaller than, or equal to, $2/\pi$, which means that as Z tends to infinity, α tends to zero.

1. INTRODUCTION AND RESULTS

As a model for a relativistic atom with nuclear charge Z and N electrons, we consider the operator

$$H_{rel} = \sum_{i=1}^{N}\left\{\sqrt{-\alpha^{-2}\Delta_i+\alpha^{-4}}-\alpha^{-2}-\frac{Z}{|x_i|}\right\}+\sum_{1\le i<j\le N}\frac{1}{|x_i-x_j|}.$$

Here, $x_i\in\mathbb{R}^3$ is the coordinate of the i'th electron, Δ_i is the Laplacian with respect to x_i, and α is Sommerfeld's fine structure constant (the physical value of α is approximately $1/137.037$). This is the expression one obtains using $\sqrt{p^2c^2+m^2c^4}-mc^2$ for the kinetic energy of the electrons (and making the substitution $p\to -i\hbar\nabla$), measuring energies (H_{rel}) in units of Rydberg, and lengths (the x_i's) in units of the Bohr radius.

This model has been much studied over the past thirty years. Stability in the case $N=1$ was proved independently by Herbst [8] and Weder [21]. The 'Stability of Matter' for the model was first proved by Conlon [2], later by Fefferman and de la Llave [6], and also by Lieb and Yau [16]; see the latter for an overview. A non-exhaustive list of other works on this model is [9, 20, 19, 18, 1].

It is well-known that the operator H_{rel} is bounded from below on $C_0^\infty(\mathbb{R}^{3N})$ if, and only if, $Z\alpha\le\frac{2}{\pi}$. Only in this case is the atom stable; and we define the operator H_{rel} as a self-adjoint, unbounded operator by Friedrichs-extending this semi-bounded operator. To study the energy of large atoms, one would normally then consider the limit as $Z\to\infty$ of the infimum of the spectrum of this operator. However, due to the upper bound on Z resulting from the restriction $Z\alpha\le\frac{2}{\pi}$, this

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is not possible here. To overcome this problem, we consider

$$H_{rel} = \alpha^{-1}\left\{\sum_{i=1}^{N}\left\{\sqrt{-\Delta_i+\alpha^{-2}}-\alpha^{-1}-\frac{\delta}{|x_i|}\right\}+\sum_{1\le i<j\le N}\frac{\alpha}{|x_i-x_j|}\right\}$$

where $\delta = Z\alpha$ is held *fixed*. This ensures that as $Z\to\infty$, and therefore $\alpha\to 0$, the operator H_{rel} remains well-defined—as long as $0\le\delta\le\frac{2}{\pi}$. Also, we shall keep $\lambda\equiv N/Z$ fixed. The energy of the atom is then defined as

$$E_N(Z,\delta) := \inf\sigma_{\mathcal{H}_F}(H_{rel})\ ,$$

where the spectrum of H_{rel} is calculated on $\mathcal{H}_F = \bigwedge^N L^2(\mathbb{R}^3,\mathbb{C}^q)$, the Fermionic Hilbert space, describing N Fermions, each with q possible spin states. We will take $q=2$ from now on (but this is no restriction). We note that since (the extension of) H_{rel} is self-adjoint and bounded from below, we have the Rayleigh-Ritz principle: If $\mathcal{C}$ is a form core for the corresponding quadratic form, then

$$\inf\sigma_{\mathcal{H}_F}(H_{rel}) = \inf_{\{\psi\in\mathcal{C}\,|\,\|\psi\|=1\}}\langle\psi, H_{rel}\psi\rangle\ .$$

Our main result is the following:

Theorem 1.1. *Let $\delta\in(0,2/\pi]$ and $\lambda>0$ be fixed and let H_{rel} and $E_{N=\lambda Z}(Z,\delta)$ be as above. Then*

$$E_{\lambda Z}(Z,\delta) = -C_{TF}(\lambda)Z^{7/3}+o(Z^{7/3})\quad,\quad Z\to\infty, \tag{1.1}$$

where $-C_{TF}(\lambda)Z^{7/3}$ is the (non-relativistic) Thomas-Fermi energy of the atom.

This shows that, to leading order, the ground-state energy of a relativistic atom is given by the (non-relativistic) semi-classical Thomas-Fermi energy approximation, as it is for the non-relativistic atom (note that the case $\delta=\frac{2}{\pi}$ is included). (In the non-relativistic case this was first proved by Lieb and Simon [13]; see also Lieb [10].) This expresses the fact that for large atoms the majority of the electrons are non-relativistic.

The second term in the expansion (1.1) will be studied in a forthcoming paper [17].

The proof of Theorem 1.1 will be by finding upper and lower bounds on $E_{\lambda Z}(Z,\delta)$. Note that the relativistic kinetic energy is always lower than the non-relativistic one:

$$\sqrt{\alpha^{-2}q^2+\alpha^{-4}}-\alpha^{-2} = \alpha^{-2}\left(\sqrt{1+(\alpha q)^2}-1\right)\le\frac{q^2}{2}. \tag{1.2}$$

(Note: since we will later make Taylor expansions of the square root in the relativistic kinetic energy, we will have to insist on the non-relativistic kinetic energy being $-\Delta/2$). This means that all upper bounds derived earlier [13, 10] for the non-relativistic operator

$$H_{cl} = \sum_{i=1}^{N}\left\{\frac{p_i^2}{2}-\frac{Z}{|x_i|}\right\}+\sum_{1\le i<j\le N}\frac{1}{|x_i-y_j|}$$

will also be upper bounds for H_{rel}; in particular, to prove Theorem 1.1, we need only derive a lower bound.

2. Organisation of the paper

We start in Section 3 by reducing the N-body operator H_{rel} to a one-particle one; having done that, we only need to consider wave functions given as Slater-determinants when trying to minimise the energy. To proceed, we need to localise the kinetic energy. To do so, we use (in Section 4) an analogue of the IMS Localisation Formula for the Schrödinger operator, see [3, p.27]. This formula has already been developed by Lieb and Yau in [16] for both the operator $\sqrt{-\Delta+\alpha^{-2}}-\alpha^{-1}$ and the hyper-relativistic kinetic energy $|p|$. This is essentially done by finding the integral kernels of these operators. For $\sqrt{-\Delta+\alpha^{-2}}-\alpha^{-1}$, this involves the modified Bessel function K_2, and the derivation of the formula and of needed properties of K_2 are carried out in Appendix A. The localisation error, given by a bounded operator $L^{(\alpha)}$ expressed as an integral operator involving K_2, is then estimated (in Section 5). Estimating the error is rather technical (calculative) and involves localisation of the operator and the above mentioned properties of K_2. Some of the localised terms are estimated with the localised energy itself (Sections 6 and 7).

Coming to the localised energy, we have to estimate the kinetic energy close to the nucleus. Since this is the high-energy region, this is where the electrons are relativistic, and so this term should be of lower order, since, to leading order, there should be no relativistic contribution to the energy. As the relativistic kinetic energy is asymptotically linear in p in the high-energy region—as opposed to the classical one which is quadratic—the singularity in the potential causes substantially more trouble. This problem is solved (in Section 6) by a clever choice of parameters in an estimate by Lieb and Yau in [16] on the sum of the eigenvalues of the energy in a ball around the nucleus. This also determines the scale on which one can localise close to the nucleus. A part of two of the localised terms of the operator $L^{(\alpha)}$ is estimated along with this term.

In the outer region, one uses (in Section 8) essentially the same idea as Lieb did in the classical case, see [11], to re-find the desired phase space integral, which is to give the semi-classical Thomas-Fermi energy. This involves introducing coherent states and estimating the error by doing so. The formulae for the relativistic case were developed in [15], but the error obtained there is too rough for our purposes. We therefore develop (in Appendix B) a better estimate by a more careful analysis. In order to make all this work, one need the coherent state to be supported further out than the initial cut-off around the nucleus. To get this, an intermediary zone is introduced (also in Section 4) by an additional cut-off. The energy in this shell is estimated (in Section 7) by a generalised version of the Lieb-Thirring inequality, proved by Daubechies in [4]. Also the other part of the previously mentioned two terms of the localised operator $L^{(\alpha)}$ is estimated in this way.

Finally we relate (in Section 8) the energy in the outer region to the Thomas-Fermi energy from the classical (that is, the Schrödinger) case. In this region, the kinetic energy is small, and using the specific scaling property of Thomas-Fermi theory allows one to make the change from the relativistic energy $\sqrt{-\alpha^{-2}\Delta+\alpha^{-4}}-\alpha^{-2}$ to the non-relativistic one, $-\Delta/2$, getting errors of the desired order.

3. Reduction to a one-particle problem

We will use the notation

$$H = \alpha H_{rel} = \sum_{i=1}^{N} \Big\{ \sqrt{-\Delta_i + \alpha^{-2}} - \alpha^{-1} - \frac{\delta}{|x_i|} \Big\} + \sum_{1\le i<j\le N} \frac{\alpha}{|x_i - x_j|}. \tag{3.1}$$

Recall that $\delta = Z\alpha$ is *fixed* and that the ground state energy of H_{rel} is to be proven to be of leading order $Z^{7/3}$. Since we wish to consider α as the free parameter, the relevant order of all error terms will be $o(\alpha^{-4/3})$. Also, we will denote the operator $\sqrt{-\Delta + \alpha^{-2}}$ by $\sqrt{p^2+\alpha^{-2}}$, and so $T(p) = \sqrt{p^2+\alpha^{-2}} - \alpha^{-1}$ will be the kinetic energy.

We start by reducing the problem from an N-particle problem to a one-particle one. This is done by using an inequality on the electron-electron interaction $\sum_{i<j} |x_i - x_j|^{-1}$, which will reduce this to a one-particle potential.

Choose a spherically symmetric function $g \in C_0^\infty(\mathbb{R}^3)$, non-negative, supported in the unit ball $B(0,1)$ of $\mathbb{R}^3$, and such that $\int g(x)^2\, d^3x = 1$. Let $\phi(x) = g(x)^2$ and let for $a > 0$ (a to be chosen later), $\phi_a(x) = a^{-3}\phi(x/a)$, so that $\int \phi_a(x)\, d^3x = 1$. Then for all $\rho : \mathbb{R}^3 \to \mathbb{R}$ we have:

$$\begin{aligned}
\sum_{1\le i<j\le N} \frac{1}{|x_i - x_j|} &\ge \sum_{1\le i<j\le N} \iint \frac{\phi_a(x-x_i)\phi_a(y-x_j)}{|x-y|}\, d^3x\, d^3y \\
&= \frac{1}{2}\sum_{i,j=1}^{N} \iint \frac{\phi_a(x-x_i)\phi_a(y-x_j)}{|x-y|}\, d^3x\, d^3y - \frac{1}{2} N \iint \frac{\phi_a(x)\phi_a(y)}{|x-y|}\, d^3x\, d^3y \\
&= \sum_{i=1}^{N} \iint \frac{\rho(y)\phi_a(x-x_i)}{|x-y|}\, d^3x\, d^3y - \frac{1}{2}\iint \frac{\rho(x)\rho(y)}{|x-y|}\, d^3x\, d^3y - c(\phi) N a^{-1} \\
&\quad + \frac{1}{2}\iint \frac{\Big(\sum_i \phi_a(x-x_i) - \rho(x)\Big)\Big(\sum_j \phi_a(y-x_j) - \rho(y)\Big)}{|x-y|}\, d^3x\, d^3y \\
&\ge \sum_{i=1}^{N} \iint \frac{\rho(y)\phi_a(x-x_i)}{|x-y|}\, d^3x\, d^3y - \frac{1}{2}\iint \frac{\rho(x)\rho(y)}{|x-y|}\, d^3x\, d^3y - c(\phi) N a^{-1}.
\end{aligned}$$

In the last inequality we used that $|x-y|^{-1}$ is of positive type (a positive kernel) since

$$\iint \frac{\overline{f(x)} f(y)}{|x-y|}\, d^3x\, d^3y = 4\pi \int \frac{|\hat f(p)|^2}{|p|^2}\, d^3p.$$

The constant $c(\phi)$ is independent of a:

$$c(\phi) = \frac{1}{2}\iint \frac{\phi(x)\phi(y)}{|x-y|}\, d^3x\, d^3y = 2\pi \int \frac{|\hat\phi(p)|^2}{|p|^2}\, d^3p.$$

Noting that (using the spherical symmetry of ϕ_a)

$$\begin{aligned}
&\iint \frac{\rho(y)\phi_a(x-x_i)}{|x-y|}\, d^3x\, d^3y = \iint \frac{\rho(y)\phi_a(z)}{|z-(x_i-y)|}\, d^3z\, d^3y \\
&= \int \rho(y)\big(\phi_a * |\cdot|^{-1}\big)(x_i - y)\, d^3y = \big(\rho * \phi_a * |\cdot|^{-1}\big)(x_i) \equiv \rho * \phi_a * |x_i|^{-1},
\end{aligned}$$

we get the operator inequality (see (3.1) for H):

$$H \geq \sum_{i=1}^{N} \Big\{ \sqrt{p_i^2 + \alpha^{-2}} - \alpha^{-1} - \frac{\delta}{|x_i|} + \alpha\, \rho * \phi_a * |x_i|^{-1} \Big\} \tag{3.2}$$
$$- \frac{\alpha}{2} \iint \frac{\rho(x)\rho(y)}{|x-y|}\, d^3x\, d^3y - \alpha\, c(\phi) N a^{-1}.$$

Having reduced the N-body operator H to a one-body operator, we only need to consider Slater-determinants when trying to minimise the energy. That is, when considering $\langle \psi, H\psi \rangle$ we need only consider those $\psi \in \mathcal{H}_F$ which are given by

$$\psi(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \det(m_i(x_j)),$$

where $m_i \in L^2(\mathbb{R}^3), i = 1, \dots, N$, are orthonormal. Note also that since $C_0^\infty(\mathbb{R}^3)$ is a core for the operator $\sqrt{p^2 + \alpha^{-2}} - \alpha^{-1} - \delta/|x|, \delta \in [0, 2/\pi]$ (see Herbst [8]), we need only consider m_i's in this space. Then, as soon as h is a one-particle operator acting on $L^2(\mathbb{R}^3)$, we have that

$$\langle \psi, \sum_{i=1}^{N} h_i \psi \rangle = \sum_{i=1}^{N} (m_i, h\, m_i).$$

Here, $\langle\ ,\ \rangle$ and $(\ ,\ )$ denote inner products in $L^2(\mathbb{R}^{3N})$, respectively $L^2(\mathbb{R}^3)$, both linear in the second variable, and h_i is h acting on the variable x_i of ψ. Also, we will use $\|\cdot\|_p$ for the norm in $L^p(\mathbb{R}^3)$.

4. Localisation of the kinetic energy

In order to treat the one-body operator in (3.2) and in particular the singularity in the Coulomb-potential—which causes considerably more trouble than in the non-relativistic case—we introduce, following Lieb and Yau [16], a partition of unity (see also Cycon, Froese, Kirsch and Simon [3, Definition 3.1]). For some $\beta \in (0, \frac{1}{2})$, let θ_1 and θ_2 be monotone positive smooth functions on $\mathbb{R}_+$, $0 \leq \theta_i \leq 1$, such that

$$\theta_1(\xi) = \begin{cases} 1 & \text{if } \xi < 1-\beta \\ 0 & \text{if } \xi > 1+\beta \end{cases}, \qquad \theta_2(\xi) = \begin{cases} 0 & \text{if } \xi < 1-\beta \\ 1 & \text{if } \xi > 1+\beta \end{cases},$$

and such that $\theta_1(\xi)^2 + \theta_2(\xi)^2 = 1$ for all $\xi \in \mathbb{R}_+$. Now define, with $8/9 < r < 1$ and $1/3 < t < 2/3$ (these choices of parameters are governed by the later analysis), the following three functions, which (for α sufficiently small) is a partition of unity in $\mathbb{R}^3$:

$$\chi_1(x) = \theta_1\Big(\frac{|x|}{\alpha^r}\Big), \quad \chi_2(x) = \theta_1\Big(\frac{|x|}{\alpha^t}\Big)\,\theta_2\Big(\frac{|x|}{\alpha^r}\Big), \quad \chi_3(x) = \theta_2\Big(\frac{|x|}{\alpha^t}\Big). \tag{4.1}$$

Then, at least for α sufficiently small, we have the picture in Figure 1.
According to Lieb and Yau [16, Theorem 9; α^{-1} corresponds to m] we have for $f \in C_0^\infty(\mathbb{R}^3)$ that

$$(f, \sqrt{p^2 + \alpha^{-2}} f) = \sum_{j=1}^{3} (f, \chi_j \sqrt{p^2 + \alpha^{-2}} \chi_j f) - (f, L^{(\alpha)} f) \tag{4.2}$$

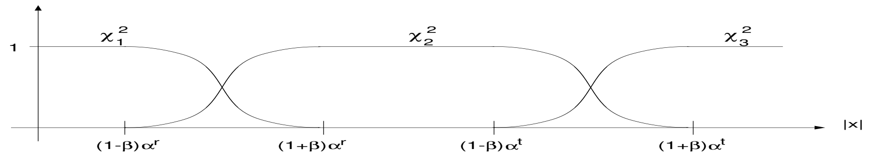

FIGURE 1. *The partition of unity.*

where $L^{(\alpha)}$ is a bounded operator on $L^2(\mathbb{R}^3)$, given by the kernel

$$L^{(\alpha)}(x,y) = \frac{\alpha^{-2}}{4\pi^2}\,\frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2}\sum_{j=1}^{3}(\chi_j(x)-\chi_j(y))^2.$$

Here K_2 is a modified Bessel-function, defined on $(0,\infty)$ by

$$K_2(t) = \frac{1}{2}\int_0^\infty x e^{-\frac{1}{2}t(x+x^{-1})}\,dx.$$

For completeness, we derive this in Appendix A.

Using this we find, with $T(p) = \sqrt{p^2+\alpha^{-2}}-\alpha^{-1}$, $V(x) = \delta/|x|$ and ψ a Slater-determinant as mentioned in the previous section, that

$$\begin{aligned}
&\langle\psi, \sum_{i=1}^{N}\big\{T(p_i) - V(x_i) + \alpha\,\rho*\phi_a*|x_i|^{-1}\big\}\psi\rangle \qquad (4.3)\\
&= \sum_{i=1}^{N}(m_i, \big\{T(p) - V(x) + \alpha\,\rho*\phi_a*|x|^{-1}\big\}m_i)\\
&= \sum_{j=1}^{3}\sum_{i=1}^{N}(m_i, \chi_j\big\{T(p) - V(x) + \alpha\,\rho*\phi_a*|x|^{-1}\big\}\chi_j m_i) - \sum_{i=1}^{N}(m_i, L^{(\alpha)}m_i),
\end{aligned}$$

since $\sum_{j=1}^3 \chi_j(x)^2 = 1$ for all $x\in\mathbb{R}^3$ (and α sufficiently small).

5. The localisation error

We now estimate the error introduced by the localisation of the kinetic energy carried out in the last section. This error is given by a bounded operator $L^{(\alpha)}$,

$$L^{(\alpha)}(x,y) = \sum_{j=1}^{3}L_j^{(\alpha)}(x,y) \quad , \quad L_j^{(\alpha)}(x,y) = \frac{\alpha^{-2}}{4\pi^2}\,\frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2}(\chi_j(x)-\chi_j(y))^2.$$

As noted above, this expression is derived in Appendix A. We shall start by localising this operator, thereby splitting it it into twelve terms (!) which we will then treat individually. These terms are going to fall into groups though, and the terms in each of these will be estimated together by different means. Two of the terms will be estimated in later sections, together with the energies near the nucleus and in the intermediary zone, related to respectively χ_1 and χ_2.

In this section, the scale of the inner cut-off will be called l, that is, $l = \alpha^r$, $8/9 < r < 1$. Let χ_- be the characteristic function of the ball $B(0,2l)$ in $\mathbb{R}^3$ and

χ_+ that for the complement of this ball. Then each $L_j^{(\alpha)}$, $j = 1,2,3$, splits into four terms:

$$L_j^{(\alpha)}(x,y) = \chi_+(x)L_j^{(\alpha)}(x,y)\chi_+(y) + \chi_+(x)L_j^{(\alpha)}(x,y)\chi_-(y) + \chi_-(x)L_j^{(\alpha)}(x,y)\chi_+(y) + \chi_-(x)L_j^{(\alpha)}(x,y)\chi_-(y).$$

The following lemma will eventually take care of six of these twelve terms:

Lemma 5.1. *Let $l = \alpha^r$, $8/9 < r < 1$ and assume that, with $\gamma \equiv 1 - \frac{b}{a} > 0$,*

$$|x| > al \quad \text{and} \quad |y| < bl \quad \text{on} \quad \operatorname{supp}\ \chi_+(x)L_j^{(\alpha)}(x,y)\chi_-(y).$$

Then, for $f \in L^2(\mathbb{R}^3)$,

$$|(f, \chi_+ L_j^{(\alpha)} \chi_- f)| \le \rho(\alpha)\|f\|_2^2\,,$$

where $\rho(\alpha) = o(e^{-2\epsilon\alpha^{r-1}})$ as $\alpha \to 0$ for all ϵ such that $0 < \epsilon < \gamma$. In particular, $\rho(\alpha) = o(\alpha^n)$ as $\alpha \to 0$ for all $n \in \mathbb{N}$.

Remark 5.2. *Note that the result with x and y interchanged also holds.*

Proof. By assumption we have that

$$|x - y| > \gamma|x| \quad \text{on} \quad \operatorname{supp}\ \chi_+ L_j^{(\alpha)}\chi_-.$$

Since both $|x|^{-2}$ and $K_2(\alpha^{-1}|x|)$ are decreasing in $|x|$ (the last is obvious from the definition of K_2), and since $(\chi_j(x) - \chi_j(y))^2 \le 1$, we get that pointwise,

$$\chi_+(x)L_j^{(\alpha)}(x,y)\chi_-(y) \le \chi_+(x)\frac{\alpha^{-2}}{4\pi^2}\frac{K_2(\alpha^{-1}\gamma|x|)}{(\gamma|x|)^2}\,\chi_-(y)$$

on supp $\chi_+ L_j^{(\alpha)}\chi_-$. Therefore

$$\begin{aligned} &|(f, \chi_+ L_j^{(\alpha)} \chi_- f)| \\ &\quad\le \left(\int |f(y)|\,\chi_-(y)\,d^3y\right)\left(\frac{(\alpha\gamma)^{-2}}{4\pi^2}\int |f(x)|\,\chi_+(x)\frac{K_2(\alpha^{-1}\gamma|x|)}{|x|^2}\,d^3x\right). \end{aligned} \tag{5.1}$$

We estimate both of these terms using the Cauchy-Schwartz inequality. For the first we get

$$\int |f(y)|\,\chi_-(y)\,d^3y \le \|f\|_2\,\|\chi_-\|_2 = Cl^{3/2}\|f\|_2, \tag{5.2}$$

and for the second

$$\int |f(x)|\,\chi_+(x)\frac{K_2(\alpha^{-1}\gamma|x|)}{|x|^2}\,d^3x \le \|f\|_2\left(\int\left(\chi_+(x)\frac{K_2(\alpha^{-1}\gamma|x|)}{|x|^2}\right)^2 d^3x\right)^{1/2}. \tag{5.3}$$

Using the estimate (A.7) in Appendix A on K_2, we get the estimate

$$\begin{aligned} &\int \left(\chi_+(x)\frac{K_2(\alpha^{-1}\gamma|x|)}{|x|^2}\right)^2 d^3x \\ &\quad\le 4\pi\int_{2l}^{\infty}\frac{16}{|x|^4}\,\frac{\pi e^{-2\alpha^{-1}\gamma|x|}}{2\alpha^{-1}\gamma|x|}\Big(1 + (2\alpha^{-1}\gamma|x|)^{-1} + (2\alpha^{-1}\gamma|x|)^{-2}\Big)^2|x|^2\,d|x| \\ &\quad= 128\pi^2\alpha^{-1}\gamma\int_{4\gamma l\alpha^{-1}}^{\infty} t^{-3}e^{-t}(1 + \frac{1}{t} + \frac{1}{t^2})^2\,dt, \end{aligned}$$

where the last equality follows by the change of variables $t = 2\gamma\alpha^{-1}|x|$. Dominating e^{-t} in the integrand by $e^{-4\gamma l\alpha^{-1}}$ and working out the resulting integral, we arrive at (using (5.1), (5.2), and (5.3); recall that $l = \alpha^r$)

$$|(f, \chi_+ L_j^{(\alpha)} \chi_- f)| \leq C\, \|f\|_2^2\, \alpha^{(3r-5)/2} e^{-2\gamma\alpha^{r-1}} \Big\{ \dots \Big\}^{1/2}$$

where

$$\Big\{ \dots \Big\}^{1/2} = \Big\{ \frac{1}{4}(4\gamma)^{-4}\alpha^{4(1-r)} + \frac{2}{5}(4\gamma)^{-5}\alpha^{5(1-r)} + \frac{1}{2}(4\gamma)^{-6}\alpha^{6(1-r)} + \frac{2}{7}(4\gamma)^{-7}\alpha^{7(1-r)} + \frac{1}{8}(4\gamma)^{-8}\alpha^{8(1-r)} \Big\}^{1/2}.$$

Now, since $8/9 < r < 1$, this term tends to zero as α tends to zero. Also

$$\alpha^{(3r-5)/2} e^{-2\gamma\alpha^{r-1}} = o(e^{-2\epsilon\alpha^{r-1}})\ ,\ \alpha \to 0,$$

for all ϵ satisfying $0 < \epsilon < \gamma$. This proves the lemma. □

We now return to investigating the above mentioned twelve terms. Firstly, note that two of these terms are actually zero:

$$\chi_+(x) L_1^{(\alpha)}(x,y)\chi_+(y) \equiv 0$$
$$\chi_-(x) L_3^{(\alpha)}(x,y)\chi_-(y) \equiv 0$$

as is easily seen by looking at the supports of χ_+, χ_-, χ_1, and χ_3. Next, we note that the following three terms fulfill the conditions in Lemma 5.1 and therefore are $o(\alpha^n), \alpha \to 0$, for all $n \in \mathbb{N}$:

$$\begin{aligned}
&\chi_+(x) L_1^{(\alpha)}(x,y)\chi_-(y) \neq 0 \quad \text{for } |x| > 2l \text{ and } |y| < (1+\beta)l \\
&\chi_+(x) L_3^{(\alpha)}(x,y)\chi_-(y) \neq 0 \quad \text{for } |x| > (1-\beta)\alpha^t \text{ and } |y| < 2l \\
&\chi_+(x) L_2^{(\alpha)}(x,y)\chi_-(y) \neq 0 \quad \text{for } |x| > (1-\beta)\alpha^t \text{ and } |y| < 2l \\
&\qquad\qquad\qquad\qquad\qquad \text{and} \quad \text{for } |x| \in [2l, (1-\beta)\alpha^t] \text{ and } |y| < (1+\beta)l.
\end{aligned}$$

This is due to the fact that for α small enough, $\alpha^t > \alpha^r$, since $t < 2/3 < 8/9 < r$. The above is symmetric in x and y, which gives another three terms.

We are then left with four terms. For these we will use that, by the Mean Value Theorem, $(\chi_j(x) - \chi_j(y))^2 \leq \|\nabla\chi_j\|_\infty^2 |x-y|^2$. Note that for the four remaining terms,

$$\chi_+ L_2^{(\alpha)} \chi_+ \quad , \quad \chi_- L_1^{(\alpha)} \chi_- \quad , \quad \chi_+ L_3^{(\alpha)} \chi_+ \quad , \quad \chi_- L_2^{(\alpha)} \chi_- \quad , \tag{5.4}$$

we only need to take the supremum of $|\nabla\chi_j(\xi)|$ over the ξ's between x and y in the support of the relevant term. In this way we get:

$$\begin{aligned}
|(f, \chi_\pm L_j^{(\alpha)} \chi_\pm f)| &\leq \iint |f(x)|\, \chi_\pm(x) |f(y)|\, \chi_\pm(y) L_j^{(\alpha)}(x,y)\, d^3x\, d^3y \\
&\leq \frac{c_j^\pm(\alpha)\alpha^{-2}}{4\pi^2} \int |f(x)|\, \chi_\pm(x) \big((|f|\, \chi_\pm) * G_\alpha \big)(x)\, d^3x
\end{aligned}$$

where $G_\alpha(x) = K_2(\alpha^{-1}|x|)$ and $c_j^\pm(\alpha) = \sup_{|x| \gtrless 2l} |\nabla\chi_j(x)|^2$. By first using the Cauchy-Schwartz inequality, then Young's inequality, we get

$$|(f, \chi_\pm L_j^{(\alpha)} \chi_\pm f)| \leq \frac{c_j^\pm(\alpha)\alpha^{-2}}{4\pi^2} \|f\,\chi_\pm\|_2\, \|\, (|f|\,\chi_\pm) * G_\alpha \|_2 \leq \frac{c_j^\pm(\alpha)}{4\pi^2\alpha^2} \|f\,\chi_\pm\|_2^2\, \|G_\alpha\|_1.$$

Since

$$\|G_\alpha\|_1 = \int K_2(\alpha^{-1}|x|)\, d^3x = 4\pi \int_0^\infty \alpha^2 t^2 K_2(t)\alpha\, dt = 6\pi^2\alpha^3$$

(see (A.6) in Appendix A for $\int_0^\infty t^2 K_2(t)\, dt$) we get the following inequality:

$$|(f, \chi_\pm L_j^{(\alpha)} \chi_\pm f)| \le \frac{3c_j^\pm(\alpha)\alpha}{2} \|f\,\chi_\pm\|_2^2. \tag{5.5}$$

For two of the terms in (5.4), $\chi_+ L_2^{(\alpha)}\chi_+$ and $\chi_+ L_3^{(\alpha)}\chi_+$, this is sufficient, since (see (4.1); recall that $l = \alpha^r$)

$$c_j^+(\alpha) = \sup_{|x|>2l} |\nabla\chi_j|^2 = c_j^+\alpha^{-2t} \quad , \quad j = 2, 3,$$

and since $t < 2/3$ we get, using (5.5), that

$$\sum_{i=1}^N (m_i, \chi_+ L_3^{(\alpha)}\chi_+ m_i) \le N\frac{3}{2}c_j^+\alpha^{1-2t} = o(\alpha^{-4/3}) \quad , \quad \alpha \to 0,$$

as $N = \lambda Z = \lambda\delta\alpha^{-1}$ (λ and δ fixed) and $\|m_i\|_2 = 1$. Similarly for $\chi_+ L_2^{(\alpha)}\chi_+$.

For the other two terms in (5.4), note that

$$\begin{aligned}\|f\,\chi_-\|_2^2 &= \int |f(x)|^2\,|\chi_-(x)|^2\, d^3x = \int |f(x)|^2\,\chi_-(x)\, d^3x = (f, \chi_- f)\\ &= (f, \chi_-(\chi_1^2 + \chi_2^2)f) = (\chi_1 f, \chi_-\chi_1 f) + (\chi_2 f, \chi_-\chi_2 f)\ ,\end{aligned}$$

since $\chi_-^2 = \chi_-$ and $\chi_1^2 + \chi_2^2 = 1$ on $\operatorname{supp}\chi_-$. Using this and (5.5), we obtain (since $\chi_-\chi_1 = \chi_1$):

$$\begin{aligned}&\sum_{i=1}^N (m_i, \chi_-(L_1^{(\alpha)} + L_2^{(\alpha)})\chi_- m_i) \qquad (5.6)\\ &\qquad \le C\,\alpha^{1-2r}\Big(\sum_{i=1}^N (\chi_1 m_i, \chi_1 m_i) + \sum_{i=1}^N (\chi_2 m_i, \chi_-\chi_2 m_i)\Big)\end{aligned}$$

where

$$C = \frac{3}{2}(c_1 + c_2) \quad , \quad c_j\alpha^{-2r} = \sup_{|x|<2l} |\nabla\chi_j(x)|^2\ ,\ j = 1, 2.$$

The two terms in (5.6) will be estimated in the following two sections, the first one along with the energy at the nucleus, the second one with the energy in the intermediary zone.

6. The energy near the nucleus

In this section we estimate the energy at the nucleus, that is (see (4.3)), the term

$$\sum_{i=1}^N (m_i, \chi_1\{T(p) - V(x) + \alpha\,\rho * \phi_a * |x|^{-1}\}\chi_1 m_i). \tag{6.1}$$

Also, half of the remaining term (5.6) of the localisation error, treated in the previous section, will be estimated here. We start by noting that $\rho * \phi_a * |x|^{-1}$ is positive, so that we get a lower bound to (6.1) by dropping this term. The remaining expression will be treated by using the following result by Lieb and Yau [16, Theorem 11] on the hyper-relativistic operator $|p|$:

Theorem 6.1. *Let $C_0 > 0$ and $R > 0$ and let*

$$H_{C_0R} = |p| - \frac{2}{\pi}|x|^{-1} - C_0/R$$

be defined on $L^2(\mathbb{R}^3)$ as a quadratic form. Let $0 \leq \gamma \leq q$ be a density matrix (that is, any bounded operator on $L^2(\mathbb{R}^3)$ which satisfies the operator inequality $0 \leq \gamma \leq q$ and for which $\mathrm{Tr}(\gamma) < \infty$) and let χ be any function with support in $B_R = \{x \,|\, |x| \leq R\}$. Then

$$\mathrm{Tr}(\bar{\chi}\gamma\chi H_{C_0R}) \geq -4.4827\, C_0^4 R^{-1} q\{(3/4\pi R^3)\int |\chi(x)|^2\, d^3x\}. \tag{6.2}$$

Note, that when $\chi \equiv 1$ in B_R, then the factor in braces $\{\}$ in (6.2) is 1.

Here, $\mathrm{Tr}(\gamma h)$ is shorthand for $\sum_k (f_k, hf_k)\gamma_k$, where (f_k, γ_k) are the eigenfunctions and eigenvalues of γ. For more details, see Lieb [12]. In our situation, $q = 2$. For our purpose, let Π be the projection on $\mathrm{span}\{m_i \,|\, i = 1, \dots N\}$, then Π is a density matrix as above, and

$$\mathrm{Tr}(\chi_1\Pi\chi_1 H_{C_0R}) = \sum_{i=1}^N (m_i, \chi_1 H_{C_0R}\chi_1 m_i).$$

Since $\mathrm{supp}\,\chi_1 \subseteq B(0, (1+\beta)\alpha^r)$ with $8/9 < r < 1$, set $R = (1+\beta)\alpha^r$ and $C_0 = 2(1+\beta)\alpha^{r-1}$. Then

$$\begin{aligned} T(p) - V(x) &= \sqrt{p^2 + \alpha^{-2}} - \alpha^{-1} - \frac{\delta}{|x|} \\ &\geq |p| - \alpha^{-1} - \frac{2}{\pi}|x|^{-1} = H_{C_0R} + \alpha^{-1}, \end{aligned}$$

since $\sqrt{p^2 + \alpha^{-2}} - \alpha^{-1} \geq |p| - \alpha^{-1}$ and $\delta \leq 2/\pi$. Including the first term in (5.6) we now have, applying (6.2),

$$\begin{aligned} &\sum_{i=1}^N (m_i, \chi_1\{T(p) - V(x)\}\chi_1 m_i) - C\,\alpha^{1-2r}\sum_{i=1}^N (m_i, \chi_1\chi_1 m_i) \\ &\qquad \geq \sum_{i=1}^N (m_i, \chi_1\{H_{C_0R} + \alpha^{-1} - C\,\alpha^{1-2r}\}\chi_1 m_i) \\ &\qquad \geq \sum_{i=1}^N (m_i, \chi_1 H_{C_0R}\chi_1 m_i) = \mathrm{Tr}(\bar{\chi}_1\Pi\chi_1 H_{C_0R}) \geq -C\alpha^{3r-4}. \end{aligned} \tag{6.3}$$

The second inequality is valid for α small enough, since $r < 1$, so that $\alpha^{2(1-r)} \to 0$ for $\alpha \to 0$. Since $3r - 4 > -4/3$ (as $8/9 < r$), the RHS of (6.3) is $o(\alpha^{-4/3})$, $\alpha \to 0$, which is the desired order. Note that the above procedure is what decides the scale α^r, $8/9 < r < 1$, on which one can localise near the nucleus.

7. The intermediary zone

The energy in this area is given by the term (see (4.3))

$$\sum_{i=1}^N (m_i, \chi_2\{T(p) - V(x) + \alpha\,\rho * \phi_a * |x_i|^{-1}\}\chi_2 m_i). \tag{7.1}$$

The zone defined by the χ_2 was introduced to separate the outer zone defined by χ_3 and the support of the coherent states to be introduced later. As in the previous section we note that by dropping the term involving $\rho * \phi_a * |x|^{-1}$, we get a lower bound of the energy in (7.1). The remaining expression will be estimated by a generalisation of the Lieb-Thirring inequality (see Lieb and Thirring [14]), proved by Daubechies in [4, page 518]. See also page 516 loc. cit. for the conditions on the function $T(p)$.

Proposition 7.1. *Let* $F(s) = \int_0^s dt\,[T^{-1}(t)]^3$, *where* $T(p) = T(|p|) = \sqrt{|p|^2 + \alpha^{-2}} - \alpha^{-1}$ *as a function. Then*

$$\langle \psi, \sum_{i=1}^N \big\{T(p_i) - V(x_i)\big\}\psi\rangle \geq\, -q\tilde{C}\int F(|V(x)|)\,d^3x$$

where $\tilde{C} \leq 0.163$.

Note that this in particular means that the negative part of the spectrum of the operator $T(p) - V(x)$ is discrete and that the sum of the negative eigenvalues of this operator is bounded from below by the quantity $-q\tilde{C}\int F(|V(x)|)\,d^3x$. To see this, let $\{e_j\}_{j=0}^\infty$ be these negative eigenvalues, $e_0 \leq e_1 \leq \dots$, and $\{g_j\}_{j=0}^\infty$ corresponding orthonormal eigenfunctions, and let ψ be the Slater-determinant of the first N of the g_j's. Then, by the above proposition,

$$\begin{aligned} -q\tilde{C}\int F(|V(x)|)\,d^3x \,&\leq \langle\psi, \sum_{i=1}^N \big\{T(p_i) - V(x_i)\big\}\psi\rangle \\ &= \sum_{j=1}^N (g_j, \big\{T(p) - V(x)\big\}g_j) = \sum_{j=1}^N e_j. \end{aligned} \tag{7.2}$$

Since the left-hand-side is independent of N, we get the statement by taking the limit $N \to \infty$. This will, as mentioned above, be used on the energy related to the cut-off χ_2, but also on the remaining half of the term $\chi_-(L_1^{(\alpha)} + L_2^{(\alpha)})\chi_-$ discussed in Section 5, see (5.6). First, let us calculate F:

$$T(p) = T(|p|) = \sqrt{|p|^2 + \alpha^{-2}} - \alpha^{-1} \Rightarrow T^{-1}(t) = \sqrt{t^2 + 2\alpha^{-1}t}.$$

Then

$$F(s) = \int_0^s (t^2 + 2\alpha^{-1}t)^{3/2}\,dt = \int_0^s \big(\frac{2t}{\alpha}\big)^{3/2}\big(1 + \frac{\alpha t}{2}\big)^{3/2}\,dt.$$

Now, by a Taylor expansion of the second term in the integral, we get

$$\big(1 + (\alpha t)/2\big)^{3/2} \leq 1 + \frac{3\alpha}{4}t + \frac{3\alpha^2}{32}t^2. \tag{7.3}$$

That is, for $s \geq 0$:

$$F(s) \leq \big(\frac{2}{\alpha}\big)^{3/2}\Big\{\frac{2}{5}s^{5/2} + \frac{3\alpha}{14}s^{7/2} + \frac{\alpha^2}{48}s^{9/2}\Big\}. \tag{7.4}$$

The two terms we wish to estimate in this section are, as mentioned above,

$$\sum_{i=1}^N (m_i, \chi_2\big\{T(p) - V(x)\big\}\chi_2 m_i) \quad \text{ and } \quad C\alpha^{1-2r}\sum_{i=1}^N (\chi_2 m_i, \chi_-\chi_2 m_i).$$

In order to do so, note that on supp $\chi_-\chi_2$ we have (χ_- being the characteristic function of $B(0, 2\alpha^r)$)

$$V(x) = \frac{\delta}{|x|} \geq \frac{\delta}{2\alpha^r} \geq C\,\alpha^{1-2r}$$

for α small enough, since $r < 1$, so that $\alpha^{1-r} \to 0$ as $\alpha \to 0$. Therefore, by the estimate (7.4) on $F(s)$, and still for α small enough, we have

$$\begin{aligned}\sum_{i=1}^{N}(m_i, \chi_2\{T(p) - V(x)\}\chi_2 m_i) - C\,\alpha^{1-2r}\sum_{i=1}^{N}(m_i, \chi_2\chi_-\chi_2 m_i)&\\ \geq \sum_{i=1}^{N}(m_i, \chi_2\{T(p) - 2\hat{V}(x)\}\chi_2 m_i)& \qquad (7.5)\end{aligned}$$

with $\hat{V}(x) = \chi_2(x)V(x)$. Letting (e_j, g_j) be the negative eigenvalues and corresponding orthonormal eigenvectors for the operator $T(p) - 2\hat{V}(x)$ as before, we then have

$$\begin{aligned}\sum_{i=1}^{N}(m_i, \chi_2\{T(p) - 2\hat{V}(x)\}\chi_2 m_i) &\geq \sum_{i=1}^{N}(\chi_2 m_i, \Big\{\sum_j e_j(g_j,\,\cdot\,)\,g_j\Big\}\,\chi_2 m_i) \qquad (7.6)\\ = \sum_j\sum_{i=1}^{N} e_j|(\chi_2 m_i, g_j)|^2 &= \sum_j\sum_{i=1}^{N} e_j|(m_i, \chi_2 g_j)|^2 \geq \sum_j e_j\|\chi_2 g_j\|^2 \geq \sum_j e_j.\end{aligned}$$

Here we used Bessel's inequality (remember that the m_i's are orthonormal), that $e_j < 0$ and that $0 \leq \chi_2 \leq 1$. Using (7.2) on $T(p) - 2\hat{V}(x)$, in the limit $N \to \infty$, we now reach (using (7.4), (7.5), and (7.6))

$$\begin{aligned}&\sum_{i=1}^{N}(m_i, \chi_2\{T(p) - V(x)\}\chi_2 m_i) - C\,\alpha^{1-2r}\sum_{i=1}^{N}(m_i, \chi_2\chi_-\chi_2 m_i)\\ &\quad\geq -2\tilde{C}\int_{\mathrm{supp}\ \chi_2} F(2\,|V(x)|)\,d^3x\\ &\quad\geq -C\int_{\mathrm{supp}\ \chi_2}\Big(\frac{2}{\alpha}\Big)^{3/2}\Big\{\frac{2}{5}\big(2|V(x)|\big)^{5/2} + \frac{3\alpha}{14}\big(2|V(x)|\big)^{7/2} + \frac{\alpha^2}{48}\big(2|V(x)|\big)^{9/2}\Big\}\,d^3x\\ &\quad= -C4\pi\int_{\alpha^r}^{\alpha^t}\Big(\frac{2}{\alpha}\Big)^{3/2}\Big\{\frac{2}{5}\big(\frac{2\delta}{|x|}\big)^{5/2} + \frac{3\alpha}{14}\big(\frac{2\delta}{|x|}\big)^{7/2} + \frac{\alpha^2}{48}\big(\frac{2\delta}{|x|}\big)^{9/2}\Big\}|x|^2\,d|x|\\ &\quad= -C\Big[\frac{4}{5}(\alpha^{\frac{t-3}{2}} - \alpha^{\frac{r-3}{2}}) + \frac{6\delta}{7}(\alpha^{\frac{-(r+1)}{2}} - \alpha^{\frac{-(t+1)}{2}}) + \frac{4\delta^2}{72}(\alpha^{\frac{1-3r}{2}} - \alpha^{\frac{1-3t}{2}})\Big].\end{aligned}$$

Since $8/9 < r < 1$ and $1/3 < t < 2/3$, all of these terms are $o(\alpha^{-4/3})$, which is the desired order. We note that it is this analysis that decides the scale α^t of the outer cut-off χ_3.

8. The outer zone and Thomas-Fermi teory

Up to order $o(\alpha^{-4/3})$ we are now left with

$$\sum_{i=1}^{N}(m_i, \chi_3\big\{T(p) - V(x) + \alpha\,\rho * \phi_a * |x|^{-1}\big\}\chi_3 m_i)$$
$$- \frac{\alpha}{2}\iint \frac{\rho(x)\rho(y)}{|x-y|}\,d^3x d^3y - \alpha\, c(\phi) N a^{-1}.$$

This expression will now be related to the semi-classical Thomas-Fermi energy. This is done by introducing coherent states, following Lieb and Yau in [15, proof of Lemma B.3]. Let g be the function chosen in Section 3, that is, $g \in C_0^\infty(\mathbb{R}^3)$, spherically symmetric, non-negative, supported in the unit ball $B(0,1)$ of $\mathbb{R}^3$ and such that $\int g(x)^2\,d^3x = 1$. Let $g_\alpha(x) = \alpha^{-3s/2} g(x/\alpha^s)$, $1/3 < t < s < 2/3$, that is, $\phi_a(x) = g_\alpha(x)^2$ with $a = \alpha^s$. In this way, since $N = \lambda Z = \lambda\delta\alpha^{-1}$:

$$\alpha\, c(\phi) N a^{-1} = \lambda\delta\, c(\phi)\alpha^{-s} = o(\alpha^{-2/3}),$$

which is also $o(\alpha^{-4/3}), \alpha \to 0$. Define now the coherent states $g_\alpha^{p,q}$, $p, q \in \mathbb{R}^3$ by

$$g_\alpha^{p,q}(x) = g_\alpha(x-q)e^{ipx}.$$

With $\tilde{T}(p)$ the function $\sqrt{p^2 + \alpha^{-2}} - \alpha^{-1}$, we then have the formulae

$$\begin{aligned}
(f,f) &= \frac{1}{(2\pi)^3}\iint d^3p\, d^3q\, (f, g_\alpha^{p,q})(g_\alpha^{p,q}, f),\\
(f,(V * g_\alpha^2)f) &= \frac{1}{(2\pi)^3}\iint d^3p\, d^3q\, V(q)(f, g_\alpha^{p,q})(g_\alpha^{p,q}, f),\\
(f, T(p)f) &\geq \frac{1}{(2\pi)^3}\iint d^3p\, d^3q\, \tilde{T}(p)(f, g_\alpha^{p,q})(g_\alpha^{p,q}, f) - o(\alpha^{-1/3}).
\end{aligned}\tag{8.1}$$

The proof of these formulae is carried out in Appendix B. In this way, letting $\tilde{V}(x) = \delta/|x| - \alpha\,\rho * |x|^{-1}$ (remember that $\phi_{\alpha^s} = g_\alpha^2$):

$$\begin{aligned}
&\sum_{i=1}^{N}(m_i, \chi_3\big\{T(p) - V(x) + \alpha\,\rho * \phi_a * |x|^{-1}\big\}\chi_3 m_i)\\
&\quad= \sum_{i=1}^{N}(m_i, \chi_3\big\{T(p) - \tilde{V}(x) * \phi_{\alpha^s} + \frac{\delta}{|x|} * \phi_{\alpha^s} - \frac{\delta}{|x|}\big\}\chi_3 m_i)\\
&\quad= \sum_{i=1}^{N}(m_i, \chi_3\big\{T(p) - \tilde{V}(x) * \phi_{\alpha^s}\big\}\chi_3 m_i)\\
&\quad= \frac{1}{(2\pi)^3}\iint d^3p\, d^3q\, \big(\tilde{T}(p) - \tilde{V}(q)\big)\Big(\sum_{i=1}^{N}|(m_i\chi_3, g_\alpha^{p,q})|^2\Big) - N\, o(\alpha^{-1/3}).
\end{aligned}$$

The second equality follows from Newton's theorem (since ϕ_{α^s} is spherically symmetric): $|x|^{-1} - |x|^{-1} * \phi_{\alpha^s} \equiv 0$ outside supp ϕ_{α^s}, and since supp $\chi_3 \cap$supp $\phi_{\alpha^s} = \emptyset$ for α sufficiently small (as $s > t$),

$$\sum_{i=1}^{N}(m_i, \chi_3\big\{\frac{\delta}{|x_i|} * \phi_{\alpha^s} - \frac{\delta}{|x_i|}\big\}\chi_3 m_i) = 0.$$

This is one of the reasons for introducing the intermediary zone by the function χ_2. Note also that $N\,o(\alpha^{-1/3}) = o(\alpha^{-4/3})$. Now, for α small enough, $\alpha^{s-t} < 1/4$, since $s > t$, so that if $|q| < \frac{1}{4}\alpha^t$, then

$$|x - q| < \alpha^s \Rightarrow |x| < \frac{1}{2}\alpha^t,$$

and so $(m_i\chi_3, g_\alpha^{p,q}) = 0$, since $\operatorname{supp}\ g_\alpha \subset B(0,\alpha^s)$ and $\operatorname{supp}\ \chi_3 \subset \mathbb{R}^3 \setminus B(0, \frac{1}{2}\alpha^t)$. That is, for α small enough

$$\operatorname{supp}_q |(m_i\chi_3, g_\alpha^{p,q})|^2 \subseteq \mathbb{R}^3 \setminus B(0, \tfrac{1}{4}\alpha^t),$$

so that for any $\mu \geq 0$ we have, with $M(p,q) = \sum_{i=1}^N |(m_i\chi_3, g_\alpha^{p,q})|^2$ and $\big[f\big]_\pm = \max\{\pm f, 0\}$:

$$\begin{aligned}
&\frac{1}{(2\pi)^3}\iint d^3p\, d^3q\, \big(\tilde{T}(p) - \tilde{V}(q)\big)\Big(\sum_{i=1}^N |(m_i\chi_3, g_\alpha^{p,q})|^2\Big) \\
&\quad = \frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac{1}{4}\alpha^t} d^3p\, d^3q\, \big(\tilde{T}(p) - (\tilde{V}(q) - \alpha\mu)\big)\, M(p,q) - \alpha\mu\sum_{i=1}^N (\chi_3 m_i, \chi_3 m_i) \\
&\quad \geq -\frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac{1}{4}\alpha^t} d^3p\, d^3q\, \Big[\tilde{T}(p) - (\tilde{V}(q) - \alpha\mu)\Big]_- - \alpha\mu N,
\end{aligned}$$

since $0 \leq M(p,q) \leq 1$ and $(\chi_3 m_i, \chi_3 m_i) \leq \|m_i\|_2^2 = 1$. The first is seen by Bessel's inequality, since the m_i's are orthonormal and $\|\chi_3 g_\alpha^{p,q}\|_2 \leq \|g_\alpha^{p,q}\|_2 = 1$. In this way we have shown that for $\mu \geq 0$, $\rho : \mathbb{R}^3 \to \mathbb{R}$ and $\psi \in \mathcal{H}_F = \bigwedge^N L^2(\mathbb{R}^3, \mathbb{C}^2)$:

$$\begin{aligned}
\langle \psi, H\psi\rangle \geq &-\frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac{1}{4}\alpha^t} d^3p\, d^3q\, \Big[\tilde{T}(p) - (\tilde{V}(q) - \alpha\mu)\Big]_- \\
&- \frac{\alpha}{2}\iint \frac{\rho(x)\rho(y)}{|x-y|}\, d^3x\, d^3y - \alpha\mu N - o(\alpha^{-4/3}).
\end{aligned} \tag{8.2}$$

Choose now ρ to be the Thomas-Fermi density $\rho_{TF}^{N,Z}$, that is, the function that minimises the Thomas-Fermi functional (here, $\gamma = (3\pi^2)^{2/3}$):

$$\mathcal{E}_{TF}(\rho) = \frac{3}{5}\gamma\int \rho(x)^{5/3}\, d^3x - \int \rho(x)\frac{Z}{|x|}\, d^3x + \frac{1}{2}\iint \frac{\rho(x)\rho(y)}{|x-y|}\, d^3x\, d^3y \tag{8.3}$$

over the set

$$\Big\{\rho \in L^{5/3}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)\,\big|\, \rho \geq 0, \int \rho(x)\, d^3x \leq N\Big\}.$$

(For the Thomas-Fermi theory, see Lieb and Simon [13] and Lieb [10]). Then $\rho_{TF}^{N,Z}$ satisfies the Thomas-Fermi equation:

$$\gamma\,\rho(x)^{2/3} = \Big[\frac{Z}{|x|} - \rho * |x|^{-1} - \mu\Big]_+ \tag{8.4}$$

for some unique $\mu = \mu(N)$. Furthermore,

$$\begin{aligned}
&\text{for } N \leq Z: \quad \int \rho_{TF}^{N,Z}(x)\, d^3x = N \quad \text{and} \quad \mu(N) > 0, \\
&\text{for } N > Z: \quad \int \rho_{TF}^{N,Z}(x)\, d^3x = Z \quad \text{and} \quad \mu(N) = 0
\end{aligned}$$

(see Lieb and Simon [13, Theorems II.17, 18 and 20]). In this way, $\int \rho_{TF}^{N,Z}(x)\,d^3x < N$ implies $N > Z$, and therefore $\mu(N) = 0$, so that we always have

$$\mu(N)\int \rho_{TF}^{N,Z}(x)\,d^3x = \mu(N)N. \tag{8.5}$$

Let $\mathcal{E}_{TF}(N,Z) \equiv \mathcal{E}_{TF}(\rho_{TF}^{N,Z})$ and define the Thomas-Fermi potential by

$$V_{TF}^{N,Z}(x) \equiv Z/|x| - \rho_{TF}^{N,Z} * |x|^{-1} - \mu(N),$$

then we have the following scaling ([13, (2.24) p.608]) (remember, that $\lambda = N/Z$ is fixed):

$$\mathcal{E}_{TF}(N,Z) = Z^{7/3}\mathcal{E}_{TF}(\lambda,1) \equiv -C_{TF}(\lambda)Z^{7/3}, \tag{8.6}$$
$$V_{TF}^{N,Z}(x) = Z^{4/3}V_{TF}^{\lambda,1}(Z^{1/3}x) \equiv Z^{4/3}V_{TF}(Z^{1/3}x). \tag{8.7}$$

The idea is now to estimate the difference between the integral in (8.2) (with $\rho = \rho_{TF}^{N,Z}$ and $\mu = \mu(N)$) and

$$-\frac{\alpha}{(2\pi)^3}\iint\limits_{|q|>\frac14\alpha^t} d^3p\,d^3q\,\Big[\frac{p^2}{2} - \big(\frac{Z}{|q|} - \rho_{TF}^{N,Z} * |q|^{-1} - \mu(N)\big)\Big]_- .$$

This is done in two steps: first, we change the domain of the integration, then we change the integrand, each time estimating the error.

First,

$$-\frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac14\alpha^t} d^3p\,d^3q\,\Big[\tilde T(p) - \alpha V_{TF}^{N,Z}(q)\Big]_- = \frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac14\alpha^t;\ \tilde T(p)<\alpha V_{TF}^{N,Z}(q)} d^3p\,d^3q\,\big(\tilde T(p) - \alpha V_{TF}^{N,Z}(q)\big)$$
$$= \frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac14\alpha^t;\ \alpha\frac{p^2}{2}<\alpha V_{TF}^{N,Z}(q)} d^3p\,d^3q\,\big(\tilde T(p) - \alpha V_{TF}^{N,Z}(q)\big) + \frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac14\alpha^t;\ \tilde T(p)<\alpha V_{TF}^{N,Z}(q)<\alpha\frac{p^2}{2}} d^3p\,d^3q\,\big(\tilde T(p) - \alpha V_{TF}^{N,Z}(q)\big).$$

Since $\tilde T(p) \ge 0$, we get

$$\iint\limits_{|q|>\frac14\alpha^t;\ \tilde T(p)<\alpha V_{TF}^{N,Z}(q)<\alpha\frac{p^2}{2}} d^3p\,d^3q\,\big(\alpha V_{TF}^{N,Z}(q) - \tilde T(p)\big) \le \alpha \iint\limits_{|q|>\frac14\alpha^t;\ \tilde T(p)<\alpha V_{TF}^{N,Z}(q)<\alpha\frac{p^2}{2}} d^3p\,d^3q\,V_{TF}^{N,Z}(q).$$

Using the scaling (8.7) and the change of variables $\omega = \delta^{1/3}\alpha^{-1/3}q$, the above is equal to

$$\delta^{1/3}\alpha^{2/3}\iint\limits_{\substack{|\omega|>\frac14\delta^{1/3}\alpha^{t-1/3}\\ \tilde T(p)<\delta^{4/3}\alpha^{-1/3}V_{TF}(\omega)<\alpha\frac{p^2}{2}}} d^3p\,d^3\omega\,V_{TF}(\omega). \tag{8.8}$$

The limits in the integral means that

$$2\delta^{4/3}\alpha^{-4/3}V_{TF}(\omega) \le p^2 \le 2\delta^{4/3}\alpha^{-4/3}V_{TF}(\omega)\big(1 + \frac12\delta^{4/3}\alpha^{2/3}V_{TF}(\omega)\big)$$

so that with

$$X = 2\delta^{4/3}\alpha^{-4/3}V_{TF}(\omega)\ ,\ Y = \frac12\delta^{4/3}\alpha^{2/3}V_{TF}(\omega)\ ,\ Z = |p|^2\ ,\ W = \frac14\delta^{1/3}\alpha^{t-1/3},$$

we have

$$
\begin{aligned}
(8.8) &= (4\pi)^2\delta^{1/3}\alpha^{2/3}\int_W^\infty d|\omega|\,|\omega|^2\,V_{TF}(\omega)\Big(\int_X^{X(1+Y)}\frac{\sqrt{Z}}{2}\,dZ\Big)\\
&= (4\pi)^2\delta^{1/3}\alpha^{2/3}\int_W^\infty d|\omega|\,|\omega|^2\,V_{TF}(\omega)\frac{X^{3/2}}{3}\big((1+Y)^{3/2}-1\big).
\end{aligned}
$$

By the Taylor-expansion (7.3), we have $(1+Y)^{3/2}\leq 1+\frac{3}{2}Y+\frac{3}{8}Y^2$, and so

$$
\begin{aligned}
(8.8) \leq C\delta^{7/3}\alpha^{-4/3}&\int_W^\infty |\omega|^2\,V_{TF}(\omega)^{5/2}\\
&\times\big(\frac{3}{4}\delta^{4/3}\alpha^{2/3}V_{TF}(\omega)+\frac{3}{32}\delta^{8/3}\alpha^{4/3}V_{TF}(\omega)^2\big)\,d|\omega|.
\end{aligned}
$$

Using that $V_{TF}^{N,Z}(x)\leq Z/|x|$, since $\mu(N)\geq 0$ and $\rho_{TF}^{N,Z}\geq 0$ (remember that $V_{TF}\equiv V_{TF}^{\lambda,1}$), we arrive at

$$
\begin{aligned}
(8.8) &\leq C\delta^{11/3}\alpha^{-2/3}\int_W^\infty d|\omega|\,|\omega|^{-3/2}+\sqrt{2}\pi^2\delta^5\int_W^\infty d|\omega|\,|\omega|^{-5/2}\\
&\sim \alpha^{-2/3}W^{-1/2}+W^{-3/2}\sim\alpha^{-2/3}\alpha^{1/6-t/2}+\alpha^{(1-3t)/2}\\
&= o(\alpha^{-5/6})+o(\alpha^{-1/2})
\end{aligned}
$$

since $t<2/3$. This means, that

$$
\begin{aligned}
-\frac{1}{(2\pi)^3}&\iint\limits_{|q|>\frac{1}{4}\alpha^t} d^3p\,d^3q\,\Big[\tilde{T}(p)-\alpha V_{TF}^{N,Z}(q)\Big]_-\\
&\geq\frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac{1}{4}\alpha^t;\ \alpha\frac{p^2}{2}<\alpha V_{TF}^{N,Z}(q)} d^3p\,d^3q\,\big(\tilde{T}(p)-\alpha V_{TF}^{N,Z}(q)\big)-o(\alpha^{-4/3}).
\end{aligned}
$$

Next note that since $|q|>\frac{1}{4}\alpha^t$ and $\alpha V_{TF}^{N,Z}(q)\leq\delta/|q|$ in the area of integration, we here have that

$$
\tilde{T}(p)=\sqrt{p^2+\alpha^{-2}}-\alpha^{-1}\geq\alpha\frac{p^2}{2}-\alpha^3\frac{p^4}{8}.
$$

In this way, we get

$$
\begin{aligned}
&\frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac{1}{4}\alpha^t;\ \alpha\frac{p^2}{2}<\alpha V_{TF}^{N,Z}(q)} d^3p\,d^3q\,\big(\tilde{T}(p)-\alpha V_{TF}^{N,Z}(q)\big)\\
&\geq\frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac{1}{4}\alpha^t;\ \alpha\frac{p^2}{2}<\alpha V_{TF}^{N,Z}(q)} d^3p\,d^3q\,\big(\alpha\frac{p^2}{2}-\alpha^3\frac{p^4}{8}-\alpha V_{TF}^{N,Z}(q)\big)\\
&=\frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac{1}{4}\alpha^t;\ \alpha\frac{p^2}{2}<\alpha V_{TF}^{N,Z}(q)} d^3p\,d^3q\,\big(\alpha\frac{p^2}{2}-\alpha V_{TF}^{N,Z}(q)\big)-\alpha^3\frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac{1}{4}\alpha^t;\ \alpha\frac{p^2}{2}<\alpha V_{TF}^{N,Z}(q)}\frac{p^4}{8}\,d^3p\,d^3q. \qquad (8.9)
\end{aligned}
$$

Note that

$$\begin{aligned}
&\frac{1}{(2\pi)^3} \iint\limits_{|q|>\frac{1}{4}\alpha^t;\ \alpha\frac{p^2}{2}<\alpha V_{TF}^{N,Z}(q)} d^3p\, d^3q \,\big(\alpha\frac{p^2}{2} - \alpha V_{TF}^{N,Z}(q)\big) \\
&= -\frac{\alpha}{(2\pi)^3} \iint\limits_{|q|>\frac{1}{4}\alpha^t} d^3p\, d^3q \,\Big[\frac{p^2}{2} - \big(\frac{Z}{|q|} - \rho_{TF}^{N,Z} * |q|^{-1} - \mu(N)\big)\Big]_- \\
&\geq -\frac{\alpha}{(2\pi)^3} \iint d^3p\, d^3q \,\Big[\frac{p^2}{2} - \big(\frac{Z}{|q|} - \rho_{TF}^{N,Z} * |q|^{-1} - \mu(N)\big)\Big]_- .
\end{aligned}$$

Let us now look at the last term in (8.9). Again using that $V_{TF}^{N,Z}(x) \leq Z/|x|$, we have that

$$\begin{aligned}
\iint\limits_{|q|>\frac{1}{4}\alpha^t;\ \alpha\frac{p^2}{2}<\alpha V_{TF}^{N,Z}(q)} \frac{p^4}{8}\, d^3p\, d^3q \;\leq\; & \iint\limits_{|q|>\frac{1}{4}\alpha^t;\ \alpha\frac{p^2}{2}<\delta/|q|} \frac{p^4}{8}\, d^3p\, d^3q \\
&= (4\pi)^2 \int_{\frac{1}{4}\alpha^t}^{\infty} d|q| \left(|q|^2 \int_0^{\sqrt{2Z/|q|}} \frac{|p|^4}{8} |p|^2\, d|p| \right) \\
&= 2\pi^2 \int_{\frac{1}{4}\alpha^t}^{\infty} d|q| \left(|q|^2 \Big[t^7/7\Big]_0^{\sqrt{2Z/|q|}} \right) \\
&= \frac{2\pi^2 (2Z)^{7/2}}{7} \int_{\frac{1}{4}\alpha^t}^{\infty} |q|^{-3/2}\, d|q| = \frac{8\pi^2(2Z)^{7/2}}{7} \alpha^{-t/2}.
\end{aligned}$$

Using this, we then get the following

$$\begin{aligned}
&\frac{1}{(2\pi)^3} \iint\limits_{|q|>\frac{1}{4}\alpha^t;\ \alpha\frac{p^2}{2}<\alpha V_{TF}^{N,Z}(q)} d^3p\, d^3q \,\big(\tilde{T}(p) - \alpha V_{TF}^{N,Z}(q)\big) \\
&\geq -\frac{\alpha}{(2\pi)^3} \iint d^3p\, d^3q \,\Big[\frac{p^2}{2} - \big(\frac{Z}{|q|} - \rho_{TF}^{N,Z} * |q|^{-1} - \mu(N)\Big]_- \\
&- \alpha^{(6-t)/2}\, \frac{(2Z)^{7/2}}{7\pi}.
\end{aligned}$$

Hence, since $\delta = Z\alpha$ is fixed and $t < 2/3$, we have

$$\alpha^{(6-t)/2}\, \frac{(2Z)^{7/2}}{7\pi} = \frac{8\sqrt{2}}{7\pi} \alpha^{-(1+t)/2} \delta^{7/2} = o(\alpha^{-4/3}) \quad , \quad \alpha \to 0.$$

Summing up, we have now proved that for $\psi \in \mathcal{H}_F = \bigwedge^N L^2(\mathbb{R}^3, \mathbb{C}^2)$:

$$\begin{aligned}
\langle \psi, H\psi \rangle \geq &-\frac{\alpha}{(2\pi)^3} \iint d^3p\, d^3q \,\Big[\frac{p^2}{2} - \big(\frac{Z}{|q|} - \rho_{TF}^{N,Z} * |q|^{-1} - \mu(N)\big)\Big]_- \\
&- \frac{\alpha}{2} \iint \frac{\rho_{TF}^{N,Z}(x) \rho_{TF}^{N,Z}(y)}{|x-y|}\, d^3x d^3y - \alpha\mu(N)N - o(\alpha^{-4/3}). \qquad (8.10)
\end{aligned}$$

Integrating firstly in p in the first integral in (8.10), we get, for each q fixed:

$$
\begin{aligned}
&\int d^3p\Big[\frac{p^2}{2}-(\frac{Z}{|q|}-\rho_{TF}^{N,Z}*|q|^{-1}-\mu(N))\Big]_- \qquad (8.11)\\
&\quad=\int\limits_{\frac{p^2}{2}<V_{TF}^{N,Z}}\Big(\frac{p^2}{2}-(\frac{Z}{|q|}-\rho_{TF}^{N,Z}*|q|^{-1}-\mu(N))\Big)d^3p=-\frac{16\sqrt{2}\pi}{15}\Big[V_{TF}^{N,Z}(q)\Big]_+^{5/2}.
\end{aligned}
$$

The $[\cdots]_+$, since, if the term in brackets is negative, the integrand in (8.11) will be zero.

Now, because $\rho_{TF}^{N,Z}$ satifies the equation (8.4), we get, that

$$
\begin{aligned}
\Big[\frac{Z}{|q|}-\rho_{TF}^{N,Z}*|q|^{-1}-\mu(N)\Big]_+^{5/2}&=\gamma^{5/2}\rho_{TF}^{N,Z}(q)^{5/3}\\
&=\gamma^{3/2}\rho_{TF}^{N,Z}(q)\Big[\frac{Z}{|q|}-\rho_{TF}^{N,Z}*|q|^{-1}-\mu(N)\Big].
\end{aligned}
$$

In the last equation, no $[\cdots]_+$ is needed, since, if the last term is negative, $\rho_{TF}^{N,Z}$ is zero, because of (8.4). In this way, by the above and by (8.5):

$$
\begin{aligned}
&-\frac{\alpha}{(2\pi)^3}\iint d^3p\,d^3q\,\Big[\frac{p^2}{2}-(\frac{Z}{|q|}-\rho_{TF}^{N,Z}*|q|^{-1}-\mu(N))\Big]_-\\
&\qquad-\frac{\alpha}{2}\iint\frac{\rho_{TF}^{N,Z}(x)\rho_{TF}^{N,Z}(y)}{|x-y|}\,d^3xd^3y-\alpha\mu(N)N\\
&=\alpha\frac{3}{5}\gamma\int\rho_{TF}^{N,Z}(q)^{5/3}\,d^3q-\alpha\int\rho_{TF}^{N,Z}(q)\frac{Z}{|q|}\,d^3q\\
&\qquad+\alpha\int\rho_{TF}^{N}(q)\,\rho_{TF}^{N,Z}*|q|^{-1}\,d^3q+\alpha\mu(N)\int\rho_{TF}^{N,Z}(q)\,d^3q\\
&\qquad-\frac{\alpha}{2}\iint\frac{\rho_{TF}^{N,Z}(x)\rho_{TF}^{N,Z}(y)}{|x-y|}\,d^3xd^3y-\alpha\mu(N)N\\
&=\alpha\left(\frac{3}{5}\gamma\int\rho_{TF}^{N,Z}(x)^{5/3}\,d^3x-\int\rho_{TF}^{N,Z}(x)\frac{Z}{|x|}\,d^3x+\frac{1}{2}\iint\frac{\rho_{TF}^{N,Z}(x)\rho_{TF}^{N,Z}(y)}{|x-y|}\,d^3x\,d^3y\right)\\
&=\alpha\,\mathcal{E}_{TF}(N,Z).
\end{aligned}
$$

Since $H_{rel}=\alpha^{-1}H$, and $Z=\delta\alpha^{-1}$, with δ fixed, $0\leq\delta\leq 2/\pi$, this shows, that for all $\psi\in\mathcal{H}_F=\bigwedge^N L^2(\mathbb{R}^3,\mathbb{C}^2)$:

$$
\langle\psi,H_{rel}\psi\rangle\geq -C_{TF}Z^{7/3}-o(Z^{7/3})\quad,\quad Z\to\infty,
$$

because of the scaling (8.6). This ends the proof of Theorem 1.1. □

Appendix A. A formula for the kinetic energy

In this appendix we shall prove the localisation-formula (4.2) for the operator $\sqrt{p^2+\alpha^{-2}}$ (which is the equivalent of the IMS Localisation Formula for the Laplace operator $-\Delta$, see Cycon, Froese, Kirsch and Simon [3, Theorem 3.2]). Let firstly K_2 be a modified Bessel-function of second order, defined on $(0,\infty)$ by

$$
K_2(t)=\frac{1}{2}\int_0^\infty xe^{-\frac{1}{2}t(x+x^{-1})}\,dx.
$$

It is easily seen that K_2 is well-defined, decreasing and differentiable. Other properties of K_2 will be derived later. Let then $\chi_j, j = 1, \ldots, k$ be smooth positive functions on $\mathbb{R}^3$, such that $\sum_j \chi_j^2(x) = 1$ for all x in $\mathbb{R}^3$ and define on $L^2(\mathbb{R}^3)$ the bounded operator $L^{(\alpha)}$ by the kernel

$$L^{(\alpha)}(x,y) = \frac{\alpha^{-2}}{(2\pi)^2} \frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2} \sum_{j=1}^{k} (\chi_j(x) - \chi_j(y))^2.$$

Then for $f \in \mathcal{S}(\mathbb{R}^3)$ one has the formula:

$$(f, \sqrt{p^2+\alpha^{-2}} f) = \sum_{j=1}^{k} (f, \chi_j \sqrt{p^2+\alpha^{-2}} \chi_j f) - (f, L^{(\alpha)} f). \tag{A.1}$$

The proof of the localisation formula (A.1) will be a consequence of the following formula:

Lemma A.1. *For $f \in \mathcal{S}(\mathbb{R}^3)$,*

$$\big(f, (\sqrt{p^2+\alpha^{-2}} - \alpha^{-1}) f\big) = \frac{\alpha^{-2}}{(2\pi)^2} \iint |f(x) - f(y)|^2 \frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2}\, d^3x\, d^3y. \tag{A.2}$$

Proof. Let $\hat{f}$ be the Fourier transform of f. Note that by dominated convergence in momentum space, we have

$$(f, \sqrt{p^2+\alpha^{-2}} f) = \lim_{t \searrow 0} \frac{1}{t} \big\{ (f,f) - (f, e^{-t\sqrt{p^2+\alpha^{-2}}} f) \big\}.$$

To calculate the integral kernel $\exp[-t\sqrt{p^2+\alpha^{-2}}](x,y)$, expand the Fourier transforms:

$$\begin{aligned}
(f, e^{-t\sqrt{p^2+\alpha^{-2}}} f) &= \int |\hat{f}(p)|^2 e^{-t\sqrt{p^2+\alpha^{-2}}}\, d^3p \\
&= \frac{1}{(2\pi)^3} \iint \overline{f(x)} f(y) \Big(\int e^{-t\sqrt{p^2+\alpha^{-2}}} e^{i(x-y)\cdot p}\, d^3p \Big)\, d^3x\, d^3y.
\end{aligned}$$

This is justified by the fact that $f \in \mathcal{S}(\mathbb{R}^3)$. Now, for x, y fixed, choose polar coordinates $(|p|, \theta, \phi)$, for p such that $(x-y)\cdot p = -|p|\,|x-y| \cos\theta$. Then

$$\begin{aligned}
&\int e^{-t\sqrt{p^2+\alpha^{-2}}} e^{i(x-y)\cdot p}\, d^3p \\
&= \int_0^\infty \int_0^{2\pi} \int_0^\pi e^{-t\sqrt{p^2+\alpha^{-2}}} e^{-i|p|\,|x-y|\cos\theta} \sin\theta\, d\theta\, d\phi\, |p|^2\, d|p| \\
&= 2\pi \int_0^\infty |p|^2 e^{-t\sqrt{p^2+\alpha^{-2}}} \Big(\int_{-1}^{1} e^{i|p|\,|x-y| u}\, du \Big)\, d|p| \quad , \quad u = -\cos\theta \\
&= \frac{4\pi}{|x-y|} \int_0^\infty |p| e^{-t\sqrt{p^2+\alpha^{-2}}} \sin(|p|\,|x-y|)\, d|p| \\
&= \frac{4\pi}{|x-y|} t\alpha^{-2} |x-y| \big(|x-y|^2 + t^2\big)^{-1} K_2\big[\alpha^{-1}(|x-y|^2+t^2)^{1/2}\big]
\end{aligned}$$

where the last equality is given in Erdelyi, Magnus, Oberhettinger and Tricomi [5, p. 75, 2.4 (35)]. In this way,

$$(f, e^{-t\sqrt{p^2+\alpha^{-2}}} f) = \frac{t\alpha^{-2}}{2\pi^2} \iint \overline{f(x)} f(y) \frac{K_2\big[\alpha^{-1}(|x-y|^2+t^2)^{1/2}\big]}{|x-y|^2+t^2} \, d^3x \, d^3y. \quad \text{(A.3)}$$

Now, letting $F_t(p) = e^{-t\sqrt{p^2+\alpha^{-2}}}$, the above shows that

$$\check{F}_t(x) = \frac{1}{(2\pi)^{3/2}} \int F_t(p) e^{ix\cdot p} \, d^3p = \sqrt{\frac{2}{\pi}} \, t\alpha^{-2} \, \frac{K_2\big[\alpha^{-1}(|x|^2+t^2)^{1/2}\big]}{|x|^2+t^2},$$

and therefore, for all $y \in \mathbb{R}^3$:

$$\frac{t\alpha^{-2}}{2\pi^2} \int \frac{K_2\big[\alpha^{-1}(|x-y|^2+t^2)^{1/2}\big]}{|x-y|^2+t^2} \, d^3x = F_t(0) = e^{-t\alpha^{-1}}. \quad \text{(A.4)}$$

Hence we get, using (A.3) and (A.4), which are both symmetric in x and y, that

$$\begin{aligned}
&\frac{1}{t}\big\{(f,f) - (f, e^{-t\sqrt{p^2+\alpha^{-2}}} f)\big\} \\
&\quad = \frac{1}{t}\big\{(f,f) - (f, e^{-t\alpha^{-1}} f)\big\} + \frac{1}{t}\big\{(f, e^{-t\alpha^{-1}} f) - (f, e^{-t\sqrt{p^2+\alpha^{-2}}} f)\big\} \\
&\quad = -\frac{e^{-t\alpha^{-1}} - e^{-0\cdot\alpha^{-1}}}{t-0} \, (f,f) \\
&\qquad + \frac{1}{t}\Big\{ \int \frac{1}{2}\Big(\big(|f(x)|^2 + |f(y)|^2\big) - \overline{f(x)} f(y) - \overline{f(y)} f(x) \Big) \\
&\qquad\qquad \times \frac{t\alpha^{-2}}{2\pi^2} \frac{K_2\big[\alpha^{-1}(|x-y|^2+t^2)^{1/2}\big]}{|x-y|^2+t^2} \, d^3x \, d^3y \Big\}.
\end{aligned}$$

Cancelling t and noting that

$$\lim_{t\searrow 0} \frac{e^{-t\alpha^{-1}} - e^{-0\cdot\alpha^{-1}}}{t-0} = \frac{d}{dt}\big(e^{-t\alpha^{-1}}\big)\Big|_{t=0} = -\alpha^{-1},$$

we get that

$$\begin{aligned}
&\lim_{t\searrow 0} \frac{1}{t}\big\{(f,f) - (f, e^{-t\sqrt{p^2+\alpha^{-2}}} f)\big\} \\
&\qquad = \alpha^{-1} + \frac{\alpha^{-2}}{(2\pi)^2} \iint |f(x) - f(y)|^2 \frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2} \, d^3x \, d^3y.
\end{aligned}$$

This proves the lemma. □

Now, to prove the formula (A.1), we simply use the fact that $\sum_j \chi_j^2(x) = 1$ for all x in $\mathbb{R}^3$:

$$\begin{aligned}
&\sum_{j=1}^{k} |\chi_j(x) f(x) - \chi_j(y) f(y)|^2 \\
&= |f(x)|^2 + |f(y)|^2 - \sum_{j=1}^{k} \chi_j(x)\chi_j(y)\big(\overline{f(y)} f(x) + \overline{f(x)} f(y)\big) \\
&= |f(x) - f(y)|^2 + \sum_{j=1}^{k} \chi_j(x)\big(\overline{f(y)} f(x) + \overline{f(x)} f(y)\big)\big(\chi_j(x) - \chi_j(y)\big).
\end{aligned}$$

Note that $\chi_j f \in \mathcal{S}(\mathbb{R}^3)$, since χ_j is smooth and bounded, so that using the formula (A.2):

$$\begin{aligned}\sum_{j=1}^k (f, \chi_j(\sqrt{p^2+\alpha^{-2}} - \alpha^{-1})\chi_j f) &= \sum_{j=1}^k (\chi_j f, (\sqrt{p^2+\alpha^{-2}} - \alpha^{-1})\chi_j f) \\ &= \frac{\alpha^{-2}}{(2\pi)^2} \iint \sum_{j=1}^k |\chi_j(x)f(x) - \chi_j(y)f(y)|^2 \, \frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2} \, d^3x \, d^3y \\ &= \frac{\alpha^{-2}}{(2\pi)^2} \iint \Big\{ |f(x)-f(y)|^2 + \sum_{j=1}^k \chi_j(x)\big(\overline{f(y)}f(x) \\ &\qquad + \overline{f(x)}f(y)\big)\big(\chi_j(x)-\chi_j(y)\big)\Big\} \frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2} \, d^3x \, d^3y. \end{aligned} \tag{A.5}$$

Using now that

$$\begin{aligned}&\iint \chi_j(x)\overline{f(y)}f(x)\big(\chi_j(x)-\chi_j(y)\big) \frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2} \, d^3x \, d^3y \\ &\quad = -\iint \chi_j(y)\overline{f(x)}f(y)\big(\chi_j(x)-\chi_j(y)\big) \frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2} \, d^3x \, d^3y\end{aligned}$$

simply by interchanging x and y, we finally get from (A.5) that

$$\begin{aligned}\sum_{j=1}^k (f, \chi_j \sqrt{p^2+\alpha^{-2}}\chi_j f) &= \frac{\alpha^{-2}}{(2\pi)^2} \iint |f(x)-f(y)|^2 \frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2} \, d^3x \, d^3y \\ &+ \frac{\alpha^{-2}}{(2\pi)^2} \iint \overline{f(x)}f(y) \sum_{j=1}^k \big(\chi_j(x)-\chi_j(y)\big)^2 \frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2} \, d^3x \, d^3y\end{aligned}$$

which, using (A.2), proves the formula (A.1). □

We now derive two facts about the function K_2:

$$\int_0^\infty t^2 K_2(t)\, dt = \frac{3\pi}{2}, \tag{A.6}$$

$$K_2(t) \le 4\sqrt{\frac{\pi}{2t}}\, e^{-t}\,\Big(1 + \frac{1}{2t} + \frac{1}{(2t)^2}\Big) \quad \text{for all } t \in \mathbb{R}_+ \tag{A.7}$$

The proof of (A.6) is straightforward by using the definition of K_2:

$$\begin{aligned}\int_0^\infty t^2 K_2(t)\, dt &= \int_0^\infty t^2 \Big(\frac{1}{2}\int_0^\infty x e^{-\frac{1}{2}(x+x^{-1})}\, dx\Big)\, dt \\ &= \frac{1}{2}\int_0^\infty x \Big(\int_0^\infty t^2 e^{-\frac{1}{2}(x+x^{-1})}\, dt\Big)\, dx\end{aligned}$$

where the interchanging of the order of integration is allowed by Tonelli's theorem. By applying partial integration three times,

$$\int_0^\infty t^2 e^{-\frac{1}{2}(x+x^{-1})}\, dt = \frac{16}{(x+x^{-1})},$$

and so

$$\begin{aligned}\int_0^\infty t^2 K_2(t)\,dt &= \frac{1}{2}\int_0^\infty \frac{16x}{(x+x^{-1})}\,dx = 4\int_{-\infty}^\infty \frac{x^4}{(x^2+1)^3}\,dx\\ &= 4\cdot 2\pi i\,\mathrm{Res}\Big(\frac{z^4}{(z^2+1)^3}, i\Big) = 8\pi i\frac{6}{32i} = \frac{3\pi}{2}.\end{aligned}$$

For the estimate (A.7), we need to rewrite K_2. This is done following Gray and Mathews [7, pp. 50].

Observation A.2.

$$K_2(t) = \sqrt{\frac{\pi}{2t}}\,\frac{1}{\Gamma(\frac{5}{2})}\,e^{-t}\int_0^\infty e^{-\xi}\xi^{3/2}\big(1+\frac{\xi}{2t}\big)^{3/2}\,d\xi. \tag{A.8}$$

To prove the observation, we start on the right-hand-side of (A.8). Setting $t+\xi = \sqrt{t^2+\eta}$, one gets, since then $\eta = \xi^2 + 2t\xi$, that

$$\mathrm{RHS}\ (A.8) = \sqrt{\frac{\pi}{2t}}\,\frac{1}{\Gamma(\frac{5}{2})}\int_0^\infty e^{-\sqrt{t^2+\eta}}\big(\frac{\eta}{2t}\big)^{3/2}\frac{d\eta}{2\sqrt{t^2+\eta}}.$$

Using the formula

$$\int_0^\infty e^{-(a^2\xi^2+b^2/\xi^2)}\,d\xi = \frac{\sqrt{\pi}}{2a}\,e^{-2ab}$$

(which holds since both sides satisfy the differential equation $df/db = -2af$, $f(b=0) = \sqrt{\pi}/2a$) with $a = \sqrt{t^2+\eta}$, $b = 1/2$, we arrive at

$$\begin{aligned}\mathrm{RHS}\ (A.8) &= \frac{1}{\Gamma(\frac{5}{2})(2t)^2}\int_0^\infty \eta^{3/2}\Big(\int_0^\infty e^{-\big((t^2+\eta)\xi^2+1/(2\xi)^2\big)}\,d\xi\Big)\,d\eta\\ &= \frac{1}{\Gamma(\frac{5}{2})(2t)^2}\int_0^\infty e^{-(t^2\xi^2+1/(2\xi)^2)}\Big(\int_0^\infty e^{-\eta\xi^2}\eta^{3/2}\,d\eta\Big)\,d\xi\\ &= \frac{1}{(2t)^2}\int_0^\infty e^{-(t^2\xi^2+1/(2\xi)^2)}\xi^{-5}\,d\xi\end{aligned}$$

since one has the formula

$$\int_0^\infty e^{-\eta\xi^2}\eta^{3/2}\,d\eta = \xi^{-5}\Gamma(\tfrac{5}{2}).$$

Making the change of variables $x = \frac{1}{2t\xi^2}$, we finally get

$$\mathrm{RHS}\ (A.8) = \frac{1}{2}\int_0^\infty x e^{-\frac{1}{2}t(x+x^{-1})}\,dx = K_2(t).$$

Now, to prove the estimate (A.7), use the Tayloer expansion (7.3) on the integrand in (A.8), to get

$$\begin{aligned}
K_2(t) &\le \sqrt{\frac{\pi}{2t}}\,\frac{1}{\Gamma(\frac52)}\,e^{-t}\int_0^\infty e^{-\xi}\xi^{3/2}\big(1+\frac{3}{4t}\xi+\frac{3}{32t^2}\xi^2\big)\,d\xi \\
&= \sqrt{\frac{\pi}{2t}}\,\frac{1}{\Gamma(\frac52)}\,e^{-t}\Big(\int_0^\infty e^{-\xi}\xi^{3/2}\,d\xi \\
&\qquad\qquad + \frac{3}{4t}\int_0^\infty e^{-\xi}\xi^{5/2}\,d\xi + \frac{3}{32t^2}\int_0^\infty e^{-\xi}\xi^{7/2}\,d\xi\Big) \\
&= \sqrt{\frac{\pi}{2t}}\,\frac{1}{\Gamma(\frac52)}\,e^{-t}\Big(\Gamma(\tfrac52)+\frac{3}{4t}\Gamma(\tfrac72)+\frac{3}{32t^2}\Gamma(\tfrac92)\Big) \\
&= \sqrt{\frac{\pi}{2t}}\,e^{-t}\big(1+\frac{15}{8t}+\frac{105}{128t^2}\big) \le 4\sqrt{\frac{\pi}{2t}}\,e^{-t}\big(1+\frac{1}{2t}+\frac{1}{(2t)^2}\big).
\end{aligned}$$

Appendix B. Introducing coherent states

In this section we will introduce coherent states and prove the formulae in section 8. The error introduced by using coherent states will also be estimated here.

Lemma B.1. *Let $g \in C_0^\infty(\mathbb{R}^3)$ be spherically symmetric, non-negative, supported in the unit ball and such that $\|g\|_2 = 1$, and let $g^{p,q}(x) = g(x-q)e^{ipx}$. Then*

$$\begin{aligned}
(f,f) &= \frac{1}{(2\pi)^3}\iint d^3p\,d^3q\,(f,g^{p,q})(g^{p,q},f) \\
(f,(V*|g|^2)f) &= \frac{1}{(2\pi)^3}\iint d^3p\,d^3q\,V(q)(f,g^{p,q})(g^{p,q},f) \\
(f,\sqrt{p^2+\alpha^{-2}}f) &\ge \frac{1}{(2\pi)^3}\iint d^3p\,d^3q\,\sqrt{p^2+\alpha^{-2}}\,(f,g^{p,q})(g^{p,q},f) \\
&\quad - 3\alpha\,\|\nabla g\|_\infty^2 \mathrm{Vol}(\mathrm{supp}\ \ g)\,\|f\|_2^2. \qquad \text{(B.1)}
\end{aligned}$$

Proof. The idea of the above formulae is to write the identity and other operators on $L^2(\mathbb{R}^3)$ as superpositions of the one-rank operators $\pi_{pq} = (\ \ ,g^{p,q})g^{p,q}$. To prove the above formulae, start with the right-hand-side of the second formula (the proof of the first formula is similar, just more simple):

$$\begin{aligned}
&\frac{1}{(2\pi)^3}\iint d^3p\,d^3q\,V(q)(f,g^{p,q})(g^{p,q},f) \qquad \text{(B.2)} \\
&= \frac{1}{(2\pi)^3}\iint d^3p\,d^3q\,V(q)\Big[\overline{\int f(y)\overline{g(y-q)}e^{-ipy}\,d^3y}\Big]\Big[\int f(x)\overline{g(x-q)}e^{-ipx}\,d^3x\Big]
\end{aligned}$$

Notice, that the function in the last brackets is $(2\pi)^{3/2}$ times the Fourier-transform of the function $F_q(x) = f(x)\overline{g(x-q)}$. In this way we get, by Parseval's formula:

$$\begin{aligned}
\text{(B.2)} &= \iint d^3p\,d^3q\,V(q)\,|\hat F_q(p)|^2 = \int d^3q\,V(q)\,\|\hat F_q\|_2^2 = \int d^3q\,V(q)\,\|F_q\|_2^2 \\
&= \int d^3q\,V(q)\Big(\int |f(x)|^2\,|g(x-q)|^2\,d^3x\Big) \\
&= \int d^3x\,|f(x)|^2\Big(\int V(q)\,|g(x-q)|^2\,d^3q\Big) = (f,(V*|g|^2)f).
\end{aligned}$$

This proves the second (and the first) formula.

To prove the formula for the operator $\sqrt{p^2+\alpha^{-2}}$, note that

$$\int g(x-q)^2\, d^3q = 1 \text{ for all } x \text{ in } \mathbb{R}^3,$$

so that, by the symmetry of the operator $\sqrt{p^2+\alpha^{-2}}$:

$$\begin{aligned}
(f, \sqrt{p^2+\alpha^{-2}}f) &= \frac{1}{2}\iint \overline{f(x)} g(x-q)^2 \big(\sqrt{p^2+\alpha^{-2}}f\big)(x)\, d^3q\, d^3x \\
&\quad + \frac{1}{2}\iint \overline{\big(\sqrt{p^2+\alpha^{-2}}f\big)(x)}\, g(x-q)^2 f(x)\, d^3q\, d^3x \\
&= \frac{1}{2}\iint \overline{f(x)} g_q(x)^2 \big(\sqrt{p^2+\alpha^{-2}}f\big)(x)\, d^3q\, d^3x \\
&\quad + \frac{1}{2}\iint \overline{f(x)} \Big(\sqrt{p^2+\alpha^{-2}}\big({g_q}^2 f\big)\Big)(x)\, d^3q\, d^3x. \qquad \text{(B.3)}
\end{aligned}$$

Here, $g_q(x) = g(x-q)$. Remembering that $g_q(x)^2$ is reel and letting ${g_q}^2$ denote the multiplication operator defined by this function, we have

$$\begin{aligned}
&\text{(B.3)} = \iint \overline{(g_q f)(x)} \big[\sqrt{p^2+\alpha^{-2}}(g_q f)\big](x)\, d^3q\, d^3x \qquad \text{(B.4)} \\
&+ \frac{1}{2}\iint \overline{f(x)} \Big[\big({g_q}^2\sqrt{p^2+\alpha^{-2}} + \sqrt{p^2+\alpha^{-2}}{g_q}^2 - 2g_q\sqrt{p^2+\alpha^{-2}}g_q\big)f\Big](x)\, d^3q\, d^3x \\
&= \frac{1}{2}\iint \overline{f(x)} \big(L_q f\big)(x)\, d^3q\, d^3x \\
&+ \iint \Big(\int \sqrt{p^2+\alpha^{-2}}\Big(\int e^{-ipy} g_q(y) f(y)\, d^3y\Big) e^{ipx}\, d^3p\Big) g_q(x)\overline{f(x)},\, d^3q\, d^3x
\end{aligned}$$

where

$$\begin{aligned}
&\big(L_q f\big)(x) = \qquad \text{(B.5)} \\
&\quad \int \Big\{ \int \big[g_q(y)^2 + g_q(x)^2 - 2g_q(x)g_q(y)\big]\sqrt{p^2+\alpha^{-2}} e^{ip(x-y)}\, d^3p \Big\} f(y)\, d^3y.
\end{aligned}$$

The second term in (B.4) is equal to

$$\begin{aligned}
&\iint d^3p\, d^3q\, \sqrt{p^2+\alpha^{-2}} \Big(\int \overline{f(x)} g_q(x) e^{ipx}\, d^3x\Big)\Big(\int f(y) g_q(y) e^{-ipy}\, d^3y\Big) \\
&= \iint d^3p\, d^3q\, \sqrt{p^2+\alpha^{-2}}\, (f, g^{p,q})(g^{p,q}, f).
\end{aligned}$$

The first term in (B.4) is the error, which will now be estimated. Keeping x and y fixed, we have, as showed in the proof of (A.2):

$$\begin{aligned}
L_q(x,y) &= \int \big[g_q(y)^2 + g_q(x)^2 - 2g_q(x)g_q(y)\big]\sqrt{p^2+\alpha^{-2}}\, e^{ip(x-y)}\, d^3p \\
&= \big[g_q(x) - g_q(y)\big]^2 \frac{\alpha^{-2}}{4\pi^2}\frac{K_2(\alpha^{-1}|x-y|)}{|x-y|^2}.
\end{aligned}$$

In this way, using the same ideas as in Section 5, we reach the estimate

$$L_q(x,y) \le \|\nabla g_q\|_\infty^2 \frac{\alpha^{-2}}{4\pi^2} K_2(\alpha^{-1}|x-y|)\big(\chi_{\operatorname{supp} g_q}(x) + \chi_{\operatorname{supp} g_q}(y)\big),$$

where $\chi_{\operatorname{supp} g_q}$ is the characteristic function of $\operatorname{supp} g_q$. This gives us that

$$\int L_q(x,y)\,d^3q \le \int \|\nabla g_q\|_\infty^2 \,\frac{\alpha^{-2}}{4\pi^2}\,K_2(\alpha^{-1}|x-y|)\,\big(\chi_{\operatorname{supp} g_q}(x) + \chi\operatorname{supp} g_q(y)\big)\,d^3q$$
$$= 2\,\|\nabla g\|_\infty^2\,\frac{\alpha^{-2}}{4\pi^2}\,K_2(\alpha^{-1}|x-y|)\operatorname{Vol}(\operatorname{supp} g).$$

By this we finally get, by using first Cauchy-Schwartz's, then Young's inequality, that

$$\begin{aligned}
&\Big|\iint \overline{f(x)} \int L_q(x,y)\,d^3q\, f(y)\,d^3x\,d^3y\Big| \\
&\le \iint |f(x)|\,\Big(2\,\|\nabla g\|_\infty^2\,\frac{\alpha^{-2}}{4\pi^2}\,K_2(\alpha^{-1}|x-y|)\operatorname{Vol}(\operatorname{supp} g)\Big)|f(y)|\,d^3x\,d^3y \\
&\le 2\,\|\nabla g\|_\infty^2\,\frac{\alpha^{-2}}{4\pi^2}\,\|f\|_2\,\||f| * G_\alpha\|_2 \operatorname{Vol}(\operatorname{supp} g) \quad,\ G_\alpha(x) = K_2(\alpha^{-1}|x|) \\
&\le \|\nabla g\|_\infty^2\,\frac{\alpha^{-2}}{2\pi^2}\,\|f\|_2^2\,\|G_\alpha\|_1 \operatorname{Vol}(\operatorname{supp} g) \\
&= \|\nabla g\|_\infty^2\,\frac{\alpha^{-2}}{2\pi^2}\,6\pi^2\alpha^3\|f\|_2^2 \operatorname{Vol}(\operatorname{supp} g) \qquad \text{(see A.6 for } \|G_\alpha\|_1) \\
&= 3\alpha\,\|\nabla g\|_\infty^2 \operatorname{Vol}(\operatorname{supp} g)\,\|f\|_2^2.
\end{aligned}$$

$\square$

For the case (8.1) in Section 8, let the coherent state $g^{p,q}$ be defined from the scaled version of the function g chosen there—that is, $g \in C_0^\infty(\mathbb{R}^3)$, spherically symmetric, non-negative and with support in the unit ball $B(0,1)$ of $\mathbb{R}^3$. Then the coherent states are

$$g_\alpha^{p,q}(x) = g_\alpha(x-q)e^{ipx} = \alpha^{-3s/2} g\big(\frac{x-q}{\alpha^s}\big)e^{ipx}.$$

In this way, $\|\nabla g_\alpha\|_\infty^2 = \alpha^{-5s}\|\nabla g\|_\infty^2$ and $\operatorname{Vol}(\operatorname{supp} g_\alpha) = \frac{4\pi}{3}\alpha^{3s}$, and therefore

$$(f, \sqrt{p^2+\alpha^{-2}}f) \ge \frac{1}{(2\pi)^3}\iint d^3p\,d^3q\,\sqrt{p^2+\alpha^{-2}}\,(f, g_\alpha^{p,q})(g_\alpha^{p,q}, f) \;-\; o(\alpha^{-1/3}),$$

since, as $s < 2/3$,

$$3\alpha\alpha^{-5s}\,\|\nabla g\|_\infty^2\,\frac{4\pi}{3}\alpha^{3s}\,\|f\|_2^2 = C\,\alpha^{1-2s} = o(\alpha^{-1/3})\ ,\ \alpha \to 0.$$

This proves the formula (8.1), since

$$(f,f) = \frac{1}{(2\pi)^3}\iint d^3p\,d^3q\,(f, g_\alpha^{p,q})(g_\alpha^{p,q}, f)$$

and $T(p) = \sqrt{p^2+\alpha^{-2}} - \alpha^{-1}$.

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