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Towards a Relativistic Scott Correction.

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Contents

1. Introduction

In this Ph.D.-thesis we continue the study of the large-Z behaviour of the ground state energy of atoms having relativistic kintetic energy $\sqrt{p^2c^2+m^2c^4}-mc^2$; this work was initiated in Sørensen [40], which was the progress-report for the qualifying exam after the 'del A' of the Ph.D.-program. This report is included in this thesis for completeness, but has already been assessed for the Master's degree ('Cand. Scient.') at the Department of Mathematics, University of Aarhus.

The aim of this work is to try to understand relativistic corrections to the ground state energy of large atoms. As a model for a relativistic atom with atom number Z and N electrons, we considered in Sørensen [40] the dimensionless operator

$$H_{rel}=\sum_{i=1}^{N}\left\{\sqrt{-\alpha^{-2}\Delta_i+\alpha^{-4}}-\alpha^{-2}-\frac{Z}{|x_i|}\right\}+\sum_{1\leq i<j\leq N}\frac{1}{|x_i-x_j|}. \tag{1.1}$$

In physical units, the operator H_{rel} has a factor of R_∞, the Rydberg-energy, the fundamental energy of atomic physics, given by $R_\infty=\frac{1}{2}\alpha^2mc^2$. Here and above, α is a dimensionless number, the 'fine structure constant', given by fundamental constants: $\alpha=\frac{e^2}{\hbar c}$. Its value is $\approx 1/137$; m is the mass of the electron, $-e$ its charge, $\hbar$ is Planck's constant and c the speed of light (see Sørensen [40, app. A] for a derivation of the expression (1.1)). As noted in the introduction to [40], this model has already been studied extensively over the years, especially the question of 'Stability of Matter' has received great attention. We refer to [40] for references.

The corresponding problem for the non-relativistic case,

$$H_{cl} = \sum_{i=1}^{N} \left\{ -\frac{\Delta_i}{2} - \frac{Z}{|x_i|} \right\} + \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|}, \tag{1.2}$$

has been much studied over the past 20 years. Define the ground state energy of the non-relativistic atom by

$$E_N^{cl}(Z) :\equiv \inf \ \mathrm{Spec}_{\mathcal{H}_F} H_{cl} \tag{1.3}$$

where the spectrum of H_{cl} 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 (the 'Pauli Principle'). We will take $q = 2$ from now on; we will also restrict ourselves to the neutral case, $N = Z$. Then the asymptotic behaviour of $E_{N=Z}^{cl}(Z)$, as $Z \to \infty$, is known in great detail:

Theorem 1.1. *With $E_N^{cl}(Z)$ as above, there exist positive constants C_{TF} and C_{DS}, such that*

$$\begin{aligned} E_{N=Z}^{cl}(Z) = -C_{TF} Z^{7/3} + \frac{1}{2} Z^2 - C_{DS} Z^{5/3} \\ + o(Z^{5/3-\epsilon}), \quad Z \to \infty \end{aligned} \tag{1.4}$$

for some positive ϵ.

(We shall not have anything further to say on the third term, the Dirac-Schwinger correction (predicted by the physicists Dirac [3] and Schwinger [29]), proved in a long series of papers by Fefferman and Seco [6, 7, 8, 9, 10, 11, 12]).

The leading order term in this expression stems from the 'bulk' part of the electrons, and is a semi-classical term; it is given by the Thomas-Fermi energy approximation. This was first proved (rigorously) by Lieb and Simon [21] (see also Lieb [19, 20]) (but stated from physical arguments by the physicists Thomas and Fermi in the early days of quantum mechanics). Since this term comes from electrons far away from the nucleus, with low momentum $|p|$, this is a non-relativistic term. Therefore one would expect that to leading order in Z, the ground state energy of a relativistic atom should be the same.

The second term in the expansion (1.4) is called the 'Scott-correction', after the physicist Scott, who predicted it in Scott [30]. Studying the proof (by Hughes [16] and Siedentop and Weikard [31, 32, 33, 34]) of this term, one sees that it comes from a purely one-particle effect. Heuristically speaking it arises as follows: the 'innermost' electron does not feel the other electrons, and therefore the major contribution to its energy should not be the semi-classical Thomas-Fermi energy. Instead, this electron should be treated quantum mechanically. Since the energy of a (Hydrogenic) atom with one electron and a nucleus of charge

Z is of the order $-Z^2$, both 'morally' and directly seen in the rigourous proof, this term comes from a refined quantum mechanical study of the sum of the negative eigenvalues of the corresponding one-particle operator . Since the 'innermost' electron has a high momentum $|p|$, this is where we would expect to detect relativistic effects. More precisely, the second order term in a corresponding asymptotic expansion of the energy of a relativistic atom should be of the same order, but (perhaps) with a different constant (for the classical case, it is a factor 1/2).

The reason why the energy of large atoms as described by the operator in (1.1) has not yet been studied at all is the following: when looking at the one-particle operator

$$\begin{aligned} h_{Herbst} &= \sqrt{-\alpha^{-2}\Delta + \alpha^{-4}} - \alpha^{-2} - \frac{Z}{|x|} \\ &= \alpha^{-1}\Big(\sqrt{-\Delta + \alpha^{-2}} - \alpha^{-1} - \frac{Z\alpha}{|x|}\Big) \end{aligned} \tag{1.5}$$

one immidiately encounters the problem, that this operator is not well-defined beyond a certain value of $Z\alpha$ — in fact, the operator is bounded from below on $C_0^\infty(\mathbb{R}^3)$ if, and only, if $Z\alpha \leq \frac{2}{\pi}$, as proved independently by Herbst [14] and Weder [43]. As mentioned, the value of α is approximately 1/137 and so this means that only physical elements with $Z \leq 87$ are well-defined within this model.

This fact also poses problems from a purely mathematical point of view, since what we wish is to study the large-Z limit of the bottom of the spectrum of H_{rel}. (It should be mentioned that apart from this, the operator suffers from other defects: it is neither local (which is normally a required feature in quantum mechanics), nor is it Lorentz-invariant (and hence does not qualify as a 'proper' relativistic operator). We shall come back to this later.)

A way to get around the mathematical part of the problem is the following: We can re-write the operator H_{rel} as follows:

$$H_{rel} = \alpha^{-1}\Big\{\sum_{i=1}^{N}\Big\{\sqrt{-\Delta_i + \alpha^{-2}} - \alpha^{-1} - \frac{\delta}{|x_i|}\Big\} + \sum_{1\leq i<j\leq N}\frac{\alpha}{|x_i - x_j|}\Big\} \tag{1.6}$$

with $\delta = Z\alpha$. Now, as long as δ stays fixed, with $0 \leq \delta \leq \frac{2}{\pi}$, this operator is well-defined and bounded from below on $\bigwedge^N C_0^\infty(\mathbb{R}^3)$ (see Lieb and Yau [23]). Defining its Friedrichs-extension, we get a self-adjoint operator (by abuse of notation also denoted by H_{rel}), and so we can define the energy of the relativistic atom described by the operator (1.1) by

$$E_N^{rel}(Z,\delta) :\equiv \inf \operatorname{Spec}_{\mathcal{H}_F} H_{rel} \tag{1.7}$$

where the spectrum of H_{rel} as before is calculated on $\mathcal{H}_F = \bigwedge^N L^2(\mathbb{R}^3, \mathbb{C}^2)$; we will restrict ourselves to the neutral case, $N = Z$.

The point is the following: keeping δ fixed, letting Z tend to infinity (and, therefore, letting the fine structure constant α, whose physical value is $\approx 1/137$, tend to zero), we can study the asymptotics of $E_N^{rel}(Z,\delta)$ as $Z \to \infty$. Observe that

$$\alpha^{-1}\big(\sqrt{p^2+\alpha^{-2}}-\alpha^{-1}\big) \approx \frac{p^2}{2} \tag{1.8}$$

for either α fixed and $|p|$ small, or $|p|$ fixed and α small. This means that in some sense we are taking a non-relativistic limit, as well as the large-Z limit. The idea is that in the limit we should still be able to detect traces of the relativistic effects described earlier.

The study of the leading order term in the large-Z asymptotics (with $\delta = Z\alpha \le 2/\pi$ fixed) of $E_{N=Z}^{rel}(Z,\delta)$ was carried out in Sørensen [40]. The following (which confirms the heuristic idea from the earlier discussion) was proved:

Theorem 1.2 (Sørensen '96). *Let δ be fixed, $0 \le \delta \le \frac{2}{\pi}$ and let H_{rel} and $E_N^{rel}(Z,\delta)$ be as above. Then we have:*

$$E_{N=Z}^{rel}(Z,\delta) = -C_{TF}Z^{7/3} + o(Z^{7/3}), \quad Z \to \infty, \tag{1.9}$$

where $-C_{TF}Z^{7/3}$ is the Thomas-Fermi energy of the 'classical' (in the sense 'non-relativistic') atom; that is, C_{TF} is the constant from (1.4).

In Sørensen [40] the following was also conjectured:

Conjecture 1.3. For all $0 \le \delta < \frac{2}{\pi}$, there is a constant $s(\delta)$ such that

$$E_N^{rel}(Z,\delta) = -C_{TF}Z^{7/3} + s(\delta)Z^2 + o(Z^2), \quad Z \to \infty\ , \tag{1.10}$$

where $s(\delta)$ satisfies

$$\lim_{\delta\to 0} s(\delta) = \frac{1}{2}.$$

The last assertion is expected because of the (vague) intuition that small δ should correspond to a non-relativistic regime, and so we should recover the non-relativistic Scott-correction in the limit as δ tends to zero.

Both the proof of the first two terms in the expansion (1.4) and of Theorem 1.2 consist of two parts:

(*1*) Reducing the many-body problem of N electrons to that of a single-particle operator.

(*2*) A careful study of the sum of the negative eigenvalues of the resulting one-particle operator.

Having reduced the problem to the study of a one-particle operator, one is left with studying the sum of negative eigenvalues of such operators. The electron-electron interaction has been de-coupled and replaced by an 'effective potential' and, because of the Pauli Principle, we must study the sum of the N lowest eigenvalues of this one-particle operator.

Since we wish to take the limit $Z \to \infty$, we are led to the study of the sum of all the negative eigenvalues.

Various techniques to treat (*1*) are fairly standard by now, and so the latest years the hard problem has been to study (*2*).

The proof of Theorem 1.2 involved writing the kinetic energy of the one-particle operator as an integral operator in configuration space. One can then localise and utilize the heuristic ideas mentioned earlier: far away from the nucleus, the approximation (1.8) holds, and the contribution from the area close to the nucleus turns out to be of lower order.

In this thesis we study the sum of the negative eigenvalues of certain one-particle operators more carefully. We shall not as of yet have anything to say on the reduction to the one-particle operator for the case of the Scott-correction.

The present work is inspired by ideas in Sobolev [38, 39], based on methods developed by Ivriĭ [17] (see also Ivriĭ [18]). It should be mentioned here that the method of the original proofs by Hughes [16] and Siedentop and Weikard [31, 32, 33, 34] relies on the exact knowledge of the eigenvalues of the non-relativistic (Schrödinger) Hydrogen atom. The eigenvalues of the operator h_{Herbst} (see (1.5)), on the other hand, are not known. The advantage of the method of Ivriĭ is that it allows one to prove the existence of the Scott-correction in (1.4), without actually having to be able to compute it (see also Sobolev [39]). In this way, the method also works for the case of the Herbst-operator. On the other hand, this means that one will not be able to actually compute $s(\delta)$ in (1.10) by the same means as in the proof of Siedentop and Weikard. Essentially, the problem boils down to studying a pseudo-differential operator on the positive half-line, and one could hope that a further study of this operator could reveal some information on the numerical value of $s(\delta)$ (see also the end of this introduction).

The main results of this thesis are the following two theorems:

Theorem 1.4. *Let $\phi \in C_0^\infty(\mathbb{R}^3)$ be a function such that $|\phi| \leq 1$ and such that*

$$\phi(x) = \begin{cases} 1 & , \quad |x| \leq 1 \\ 0 & , \quad |x| \geq 2. \end{cases}$$

Let $\delta < 2/\pi$ be fixed, and define $\phi_t(x) = \phi(x/t)$.

Then there exists a constant $G(\delta)$, such that for any $\epsilon > 0$:

$$\begin{aligned} \operatorname{Tr}\Big\{\phi_{Z^{-1+\epsilon}}(x)\Big|\sqrt{-\alpha^{-2}\Delta_x + \alpha^{-4}} - \alpha^{-2} - \frac{Z}{|x|}\Big|_-\Big\} \\ = \frac{1}{(2\pi)^3}\iint d^3x\, d^3p\, \big(\phi_{Z^{-1+\epsilon}}(x)\big)\Big[\frac{p^2}{2} - \frac{\delta}{|x|}\Big]_- \\ + G(\delta)Z^2 + o(Z^2) \quad , \quad Z \to \infty. \end{aligned}$$

Remark 1.5. Note that the function $\phi_{Z^{-1+\epsilon}}$ is a localisation in a ball of radius $Z^{-1+\epsilon}$.

The next theorem exhibits a different way of characterising the constant $G(\delta)$:

Theorem 1.6. *Let $f(Z)$ be any strictly positive function such that $f(Z) = o(Z^2)$ as $Z \to \infty$, and let $\delta < 2/\pi$ be fixed. Then, with $G(\delta)$ the constant from Theorem 1.4:*

$$\lim_{Z\to\infty} Z^{-2}\Bigg|\mathrm{Tr}\Big\{\big|\sqrt{-\alpha^{-2}\Delta_x+\alpha^{-4}}-\alpha^{-2}-\frac{Z}{|x|}+f(Z)\,\big|_{-}\Big\} \\ -\frac{1}{(2\pi)^3}\iint d^3x\,d^3p\,\Big[\frac{p^2}{2}-\frac{\delta}{|x|}+g(Z)\Big]_{-}-G(\delta)Z^2\Bigg| = 0.$$

The aim of the future work is to extend these results to the Thomas-Fermi potential by the techniques developed in this thesis. We expect to have done most of the 'foot-work' to carry this analysis through. Finally, this should be applied to the many-body problem, to prove Conjecture 1.3.

Lastly, a note on the choice of relativistic operator. As mentioned earlier, the operator (1.5) suffers from two defects: it is neither local nor Lorentz-invariant. These two defects are not shared by the Dirac-operator, acting in $\left[C_0^\infty(\mathbb{R}^3)\right]^4$ (see Thaller [41, (4.15) p. 109; note the sign error]); its dimensionless expression is (substracting the rest mass as for h_{Herbst}):

$$h_{Dirac} = \alpha^{-1}\boldsymbol{\alpha}\cdot(-i\nabla)+\alpha^{-2}(\beta-\mathbf{1_4})-\frac{Z}{|x|}\,\mathbf{1_4} \qquad (1.11)$$

with

$$\beta = \begin{pmatrix}\mathbf{1_2} & \mathbf{0}\\ \mathbf{0} & -\mathbf{1_2}\end{pmatrix}, \quad \alpha_i = \begin{pmatrix}\mathbf{0} & \sigma_i\\ \sigma_i & \mathbf{0}\end{pmatrix}, \quad i=1,2,3,$$

where σ_i, $i=1,2,3$ are the Pauli spin-matrices:

$$\sigma_1 = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad \sigma_2 = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \quad \sigma_3 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}.$$

(We apologise to the reader for the fact that in the relativistic framework, having both α and $\boldsymbol{\alpha}$ may cause some confusion; since this is standard notation this nuissance is inevitable). This operator turns out to allow stable one-electron atoms up to $Z < 137$ (that is, $Z\alpha < 1$). This operator on the other hand suffers from the defect that it has essential spectrum $]-\infty, -mc^2]\cup[mc^2,\infty[$, which makes it impossible to define a many-body theory for this operator in a meaningfull way (we refer to recent works by Evans, Perry and Siedentop [5] and Tix [42] as attempts to remedy this problem).

One advantage of the Hydrogen Dirac-operator above is the fact that its eigenvalues are computable (Thaller [41, (7.140) p. 214]):

$$E_{n,k}^{Dirac} = \frac{Z^2}{\delta^2}\left[\left\{1+\frac{\delta^2}{(n+\sqrt{k^2-\delta^2})^2}\right\}^{-\frac{1}{2}} - 1\right],$$
$$n = 1, 2, \ldots \quad , \quad k = \pm 1, \pm 2, \ldots .$$

Assume that the leading order of the sum of these negative eigenvalues is the same as in the non-relativistic case (and therefore as in the case of the Herbst-operator in (1.5)). The eigenvalues of the (non-relativistic) Schrödinger operator are

$$E_{n,k}^{Schr} = -\frac{Z^2}{(n+k)^2}.$$

Inspired by the result of Theorem 1.6, define

$$K(\delta,\epsilon) = \frac{1}{Z^2}\left\{\sum_{E_{n,k}^{Dirac}\leq -\epsilon}\left(E_{n,k}^{Dirac}+\epsilon\right) - \sum_{E_{n,k}^{Schr}\leq -\epsilon}\left(E_{n,k}^{Schr}+\epsilon\right)\right\}$$

(taking into account the degeneracy). Then $K(\delta) = \left(\lim_{\epsilon\to 0} K(\delta,\epsilon)\right) + 1/2$ should give the first order correction, corresponding to the constant from Theorem 1.6 for the operator (1.5).

On the graph below is shown numerical values of $K(\delta,\epsilon)+1/2$ (for some small ϵ) as a function of δ, computed by Maple© (the code is included in appendix G). Note the asymptotics at $\delta \sim 0$; notice also the apparent divergence at $\delta = 1$. (Remark that the Dirac operator is well-defined for $\delta < 1$).

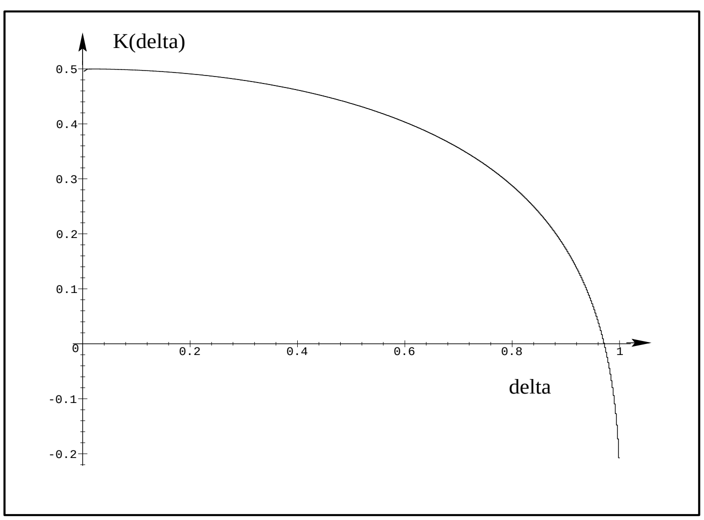

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FIGURE 1. *A numerical computation of $K(\delta)$ for Dirac.*

2. Organisation of the paper

A large deal of technical and referential material has been deferred to a number of appendicies, in order to make the exposition of the main material (closer to) linear.

In section 3 we fix some notation, then we start in section 4 by studying a one-parameter family of symbols of so-called '$h-$pseudo-differential operators' (see appendix A for referential material on the general theory of these). The family we study is, for $\alpha \in]0, \alpha_0]$:

$$a_\alpha(x,p) = \sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1} + V(x) \quad , \quad V \in C_0^\infty(\mathbb{R}^3)$$

with $p = -i\beta\nabla$ for $\beta \in]0, \beta_0]$; here, β plays the rôle of a 'small paramter'. We show that this is a symbol uniformly in α, which allows us to apply the results from appendix A, uniformly in α.

In section 5 we establish a 'modelproblem' (or a 'reference problem'), namely that of the asymptotic expansion (in β above) of $\mathrm{Tr}\{\psi\, g(A)\}$. Here, $\psi \in C_0^\infty(\mathbb{R}^3)$, with $\operatorname{supp}\psi \subset B(0, E/2)$ (an open ball of radius $E/2$) and an 'abstract' operator A, 'equal to H in $B(4E)$', with H the quantisation of the symbol a_α above, in a sense expressed in Assumption 5.1. The function g is supposed to belong to an abstract class of functions (see (5.3)), which in particular contains the functions

$$g_s(\lambda) = \begin{cases} |\lambda|^s, & \lambda < 0 \\ 0, & \lambda \geq 0 \end{cases} .$$

The asymptotics of $\mathrm{Tr}\{\psi\, g(A)\}$, expressed in Theorem 5.4, has as leading term the so-called 'Weyl-term':

$$\mathfrak{W}_{rel}(\psi, g) = \frac{1}{(2\pi\beta)^3} \int \psi(x)\, g(a_\alpha(x,p))\, d^3x\, d^3p. \tag{2.1}$$

The result is subject to a 'non-critical' condition on the symbol a_α (which translates into one on the potential V, see (5.7)). The result relies on comparing the 'abstract' operator A and the pseudo-differential operator H. This is very technical, and the results on this analysis are gathered in appendix B.

In section 6 this non-critical condition is removed by the method of Multi-scale Analysis, invented by Ivriĭ [17, 18] (see also Sigal [35] for a good account on this procedure). This method allows one to scale away the non-critical condition mentioned above in the particular case of the functions g_s mentioned above. It also allows an explicit control of the remainders, and extends to more general domains than open balls. We note here that we have not been able as of yet to carry this analysis completely through: we only prove this for the case g_1. As discussed in appendix D, we expect to be able to show the estimates in appendix B without a loss of factors of α, which will make the use of an a priori estimate (namely (D.47), proved in appendix D) in the proof of Theorem 6.7 superfluous.

The main theorems of the thesis, Theorem 1.4 and Theorem 1.6, are then proved in section 7. To this are used the results mentioned above, in a spherical shell, $\{a \leq |x| \leq b\}$, for $\alpha = \beta = 1$. Three other important ingredients come into play.

The first one is the comparing of two operators with different potentials: one being the asymptotic part as $|x| \to 0$ of the other (see appendix C). This is applied to a rather trivial case, namely that of the Coulomb potential plus a constant. The aim of future work is to extend this technique to compare the Coulomb potential with the Thomas-Fermi potential (which asymptotically as $|x| \to 0$ behaves like the Coulomb potential, see Lieb and Simon [21]).

The second important ingredient is an energy estimate of the energy of the 'tail' of all the eigenfunctions corresponding to the negative eigenvalues of a Herbst-operator, with Coulomb potential 'pushed up', see appendix E.

The last important ingredient is comparing the relativistic Weyl-term (see (2.1) above) with the 'classical' one (in the sense, 'non-relativistic'). It is important to note, that the Weyl-term entering in the two main theorems, Theorem 1.4 and Theorem 1.6, is that of the 'classical' operator (the Schrödinger operator), namely

$$\mathfrak{W}_{cl}(\phi) = \frac{1}{(2\pi)^3} \iint d^3x\, d^3p\; \phi(x) \left[\frac{p^2}{2} - \frac{\delta}{|x|}\right]_- . \tag{2.2}$$

This comparing is needed away from the singularity of the Coulomb potential. In this region, the potential, and hence the momentum $|p|$, is small, and so the relativistic kinetic energy $\sqrt{p^2+1} - 1$ is comparable to the classical kinetic energy $p^2/2$.

3. Notation

We fix some notation: for any $\eta = (\eta_1, \eta_2, \eta_3) \in \mathbb{N}^3$ and $x = (x_1, x_2, x_3) \in \mathbb{R}^3$, we denote $|\eta| = \eta_1 + \eta_2 + \eta_3$, $\eta! = \eta_1!\eta_2!\eta_3!$, $x^\eta = x_1^{\eta_1} x_2^{\eta_2} x_3^{\eta_3}$ and

$$\partial^\eta = \partial_x^\eta = \frac{\partial^{|\eta|}}{\partial x_1^{\eta_1} \partial x_2^{\eta_2} \partial x_3^{\eta_3}}.$$

We also write $\partial_l \chi = \frac{\partial \chi}{\partial x_l}$, $l = 1, 2, 3$, for brevity.

For $z \in \mathbb{R}^3$ and $\rho > 0$, we will denote the (open) ball with centre z and radius ρ by $B(z,\rho) = \{x \in \mathbb{R}^3 \mid |x - z| < \rho\}$, and $B(\rho) = B(0,\rho)$. Sometimes we write $B_p(z,\rho)$ for balls in $\mathbb{R}^3_p$; balls in $\mathbb{R}^3_x \times \mathbb{R}^3_p$ will be denoted $B_{x,p}(z,\rho)$.

By $\mathcal{B}^\infty(\mathbb{R}^3)$ we denote C^∞- functions on $\mathbb{R}^3$, which are bounded, along with all their derivatives.

The most important notation will be that of the Neumann-Schatten spaces $\mathfrak{S}_p$, trace ideals of the compact operators. These are the spaces of bounded operators T on $L^2(\mathbb{R}^3)$ such that the norm

$$\|T\|_p = \Big(\mathrm{Tr}\{(T^*T)^{\frac{p}{2}}\}\Big)^{\frac{1}{p}}$$

is finite; $\mathfrak{S}_1$, $\mathfrak{S}_2$ are the ideals of trace class operators, and Hilbert-Schmidt class operators, respectively. We note the very important fact that for $T_1 \in \mathfrak{S}_p$, $T_2 \in \mathfrak{S}_q$, and T_0 a bounded operator, we have the inequalities

$$\|T_1 T_2\|_r \le \|T_1\|_p \|T_2\|_q \quad , \quad \frac{1}{r} = \frac{1}{p} + \frac{1}{q},$$

and

$$\|T_0 T_1\|_p \le \|T_0\| \, \|T_1\|_p. \tag{3.1}$$

The first inequality extends, by induction, to what we will call 'the generalised Hölder inequality': If $T_j \in \mathfrak{S}_{p_j}$, $j = 1, \ldots, n$, then

$$\Big\| \prod_{j=1}^n T_j \Big\|_t \le \prod_{j=1}^n \|T_j\|_{p_j} \quad , \quad \frac{1}{t} = \sum_{j=1}^n \frac{1}{p_j}. \tag{3.2}$$

For more on the ideals $\mathfrak{S}_p$, we refer the reader to the monographs by Dunford and Schwartz [4], Schatten [28], and Simon [36]

For an operator T on $L^2(\mathbb{R}^3)$, $\mathcal{D}(T)$ will denote the domain of T, and for z in the resolvent set of T (that is, the complement of the spectrum of T), $R(z,T) = (T-z)^{-1}$ will be the resolvent of T at the point z. If T is semi-bounded from below, the associated quadratic form will be denoted $T[\,\cdot\,,\,\cdot\,]$ and its domain by $\mathcal{D}[T]$.

By the notation

$$f(x,y,\ldots) = g(x,y,\ldots) + \mathcal{O}(h(x,y,\ldots))$$

we mean that there exists a constant C such that

$$\big|f(x,y,\ldots) - g(x,y,\ldots)\big| \le C\, h(x,y,\ldots)$$

for $x, y, \ldots$ in some specified intervals.

Finally, for any function f, we define $|f|_\pm = \frac{1}{2}(|f| \pm f) = \max\{\pm f, 0\}$; in this way, $|f|_\pm \ge 0$. In particular, when studying the sum of the negative eigenvalues of an operator T, we need to study $\mathrm{Tr}\{-|T|_-\}$.

4. The symbol $\sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1} + V(x)$

In this section we study the symbol needed for our semi-classical analysis. This symbol will look a bit strange at first sight, but it will later become apparent why we make this unconventional choice. The reason we choose the somewhat strange looking symbol and quantisation is that this will make the 'Multi-scale Analysis' (due to Ivriĭ [17]; see also Ivriĭ [18]) in Sobolev [38, ch. 5] go through with hardly any changes.

For some $\alpha_0 > 0$ fixed, define for $\alpha \in]0, \alpha_0]$ and $V \in C_0^\infty(\mathbb{R}^3)$ on $\mathbb{R}^3_x \times \mathbb{R}^3_p$ the function

$$a_\alpha(x,p) = \sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1} + V(x).$$

With this choice of symbol, quantising by $p \to -i(\sqrt{\alpha})\nabla \equiv -i\beta\nabla$ we get the operator $\sqrt{-\Delta + \alpha^{-2}} - \alpha^{-1} + V(x)$; note also, that for small α, the symbol is approximately $p^2/2 + V(x)$, since

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

This symbol quantises to the operator $-\alpha\Delta/2 + V(x)$. In this way, whenever we get semi-classical estimates, all we have to remember is that the semi-classical parameter β is $\sqrt{\alpha}$, and not, as usual, h.

We now prove that the symbol a_α satisfies the requirements given in appendix A, uniformly in the parameter α.

Lemma 4.1. *There exist constants $b, c \geq 0$, independent of $\alpha \in]0, \alpha_0]$, such that*

$$a_\alpha + b \geq c > 0$$

and such that a_α is a weight, uniformly in the parameter $\alpha \in]0, \alpha_0]$; that is, there exists a constant C, independent of $\alpha \in]0, \alpha_0]$ (but depending on α_0, b, c and $\|V\|_\infty$) such that

$$a_\alpha(x,p) + b \leq C(1 + |x-y|^2 + |p-q|^2)(a_\alpha(y,q) + b)$$

for all (x,p) and (y,q) in $\mathbb{R}^3_x \times \mathbb{R}^3_p$ and all $\alpha \in]0, \alpha_0]$. Furthermore, a_α is a symbol with weight $a_\alpha + b$, uniformly in $\alpha \in]0, \alpha_0]$ in the sense that for all $\gamma, \eta \in \mathbb{N}^3$,

$$|\partial_x^\gamma \partial_p^\eta a_\alpha(x,p)| \leq C' x\,(a_\alpha(x,p) + b)$$

for all $(x,p) \in \mathbb{R}^3_x \times \mathbb{R}^3_p$, with a constant C' depending on γ, η, α_0, b, c and V, but independent of $\alpha \in]0, \alpha_0]$.

Proof. Firstly, since $V \in C_0^\infty(\mathbb{R}^3)$, we can, for any $c > 0$, choose a $b \geq 0$, independent of α, such that

$$a_\alpha(x,p) + b \geq c > 0 \text{ for all } x, p \in \mathbb{R}^3;$$

it suffices to take $b = b_1 + c$, with $b_1 \geq \|V\|_\infty$, since the kinetic energy, $\sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1}$, is non-negative. Next, we prove that $a_\alpha + b$ is a weight, as defined in (A.1) in appendix A. Note first that

$$\begin{aligned} a_\alpha(x,p) &= \frac{\left(\sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1}\right)\left(\sqrt{\alpha^{-1}p^2 + \alpha^{-2}} + \alpha^{-1}\right)}{\left(\sqrt{\alpha^{-1}p^2 + \alpha^{-2}} + \alpha^{-1}\right)} + V(x) \\ &= \frac{p^2}{\sqrt{\alpha p^2 + 1} + 1} + V(x) \leq p^2/2 + V(x). \end{aligned}$$

Then, for $|p| \geq 2|q|$ and any $x, y \in \mathbb{R}^3$ we have that

$$\frac{a_\alpha(x,p)+b}{1+|x-y|^2+|p-q|^2} \leq \frac{p^2/2+\|V\|_\infty+b}{1+p^2/4} \leq \max\{2, \|V\|_\infty+b\} = C_0.$$

Since $a_\alpha(y,q)+b \geq c$, we have, with $C_1 = C_0/c$ independent of α, and still for $|p| \geq 2|q|$, that

$$a_\alpha(x,p)+b \leq C_1(1+|x-y|^2+|p-q|^2)(a_\alpha(y,q)+b).$$

Next, for $|p| \leq 2|q|$, note that

$$\frac{\sqrt{\alpha^{-1}p^2+\alpha^{-2}}-\alpha^{-1}}{\sqrt{\alpha^{-1}q^2+\alpha^{-2}}-\alpha^{-1}} = \frac{|p|}{|q|}\,\frac{\sqrt{\alpha+1/|q|^2}+1/|q|}{\sqrt{\alpha+1/|p|^2}+1/|p|} \leq 4$$

since, by the above,

$$\sqrt{\alpha^{-1}p^2+\alpha^{-2}}-\alpha^{-1} = \frac{p^2}{\sqrt{\alpha p^2+1}+1},$$

and so

$$\begin{aligned}
a_\alpha(x,p)+b &= \sqrt{\alpha^{-1}p^2+\alpha^{-2}}-\alpha^{-1}+V(x)+b \\
&\leq 4\big(\sqrt{\alpha^{-1}q^2+\alpha^{-2}}-\alpha^{-1}+V(x)+b\big) \\
&= 4\big(\sqrt{\alpha^{-1}q^2+\alpha^{-2}}-\alpha^{-1}+V(y)+b+(V(x)-V(y)\big) \\
&\leq 4\big(a_\alpha(y,q)+b+2\|V\|_\infty\big) \\
&\leq 4\big(1+\frac{2\|V\|_\infty}{c}\big)\big(a_\alpha(y,q)+b\big) \\
&\leq C_2\big(1+|x-y|^2+|p-q|^2\big)\big(a_\alpha(y,q)+b\big),
\end{aligned}$$

with $C_2 = 4(1+\frac{2\|V\|_\infty}{c})$. Here we used that $V(x)+b \geq 0$ and that $a_\alpha + b \geq c$. This proves that there exists a constant C, independent of $\alpha \in]0,\alpha_0]$, such that for all $x,y,p,q \in \mathbb{R}^3$ and $\alpha \in]0,\alpha_0]$:

$$a_\alpha(x,p)+b \leq C\big(1+|x-y|^2+|p-q|^2\big)\big(a_\alpha(y,q)+b\big),$$

and so $a_\alpha + b$ is a weight as defined in (A.1) in appendix A, uniformly in α.

Next, we wish to show that a_α is a symbol of weight $a_\alpha+b$, uniformly in $\alpha \in]0,\alpha_0]$, in the sense stated in the lemma. Obviously, $a_\alpha(x,p) \leq a_\alpha(x,p)+b$ and for $\gamma \neq 0$,

$$|\partial_x^\gamma a_\alpha(x,p)| = |\partial_x^\gamma V(x)|$$

is bounded by a constant only depending on V and γ, since $V \in C_0^\infty(\mathbb{R}^3)$. Since $a_\alpha + b \geq c$ and $\partial_p^\eta \partial_x^\gamma a_\alpha = 0$ for $|\eta| \neq 0 \neq |\gamma|$, this means that we are left with bounding

$$\big|\partial_p^\eta(\sqrt{\alpha^{-1}p^2+\alpha^{-2}})\big| \quad , \quad \eta \in \mathbb{N}^3,$$

by $a_\alpha(x,p)+b$, for $\eta \neq 0$. Now, for $|\eta| = 1$, we have to bound by $a_\alpha(x,p)+b$, whereas for the higher derivatives, $|\eta| \geq 2$, it turns out that these are actually bounded uniformly in x and p. Note that, with $l = 1, 2, 3$,

$$|\partial_{p_l} a_\alpha(x,p)| = \frac{|p_l|}{\sqrt{\alpha p^2+1}} \le \frac{|p|}{\sqrt{\alpha p^2+1}}.$$

Now, for $|p| \ge 2$, we have that

$$\begin{aligned}\frac{|p|}{\sqrt{\alpha p^2+1}} &\le \frac{p^2}{2\sqrt{\alpha p^2+1}} = \frac{p^2}{\sqrt{\alpha p^2+1}+\sqrt{\alpha p^2+1}}\\ &\le \frac{p^2}{\sqrt{\alpha p^2+1}+1} = \sqrt{\alpha^{-1}p^2+\alpha^{-2}} - \alpha^{-1},\end{aligned}$$

whereas for $|p| \le 2$, the derivative is bounded:

$$\frac{|p|}{\sqrt{\alpha p^2+1}} \le |p| \le 2.$$

Since $a_\alpha + b \ge c$ and $\sqrt{\alpha^{-1}p^2+\alpha^{-2}} - \alpha^{-1} \le a_\alpha(x,p) + b$, this means that

$$|\partial_{p_l} a_\alpha(x,p)| \le C\left(a_\alpha(x,p)+b\right)$$

with $C = \max\{1, 2/c\}$.

Consider now the higher derivatives; as mentioned above

$$\partial_p^\eta a_\alpha(x,p) = \partial_p^\eta\big(\sqrt{\alpha^{-1}p^2+\alpha^{-2}}\big), \quad |\eta| \ne 0.$$

Now,

$$\sqrt{\alpha^{-1}p^2+\alpha^{-2}} = \alpha^{-1}\sqrt{1+(\sqrt{\alpha}p)^2},$$

and so

$$\partial_p^\eta\big(\sqrt{\alpha^{-1}p^2+\alpha^{-2}}\,\big) = \alpha^{-1+|\eta|/2}\big(\partial_q^\eta g\big)(\sqrt{\alpha}p) \tag{4.1}$$

with $g(q) = \sqrt{1+q^2}$. Since $\alpha \in]0, \alpha_0]$ and $|\eta| \ge 2$, it will be enough to bound $\partial_q^\eta g(q)$, uniformly in q, as $\alpha^{-1+|\eta|/2} \le \alpha_0^{(|\eta|-2)/2}$.

To do this we will prove the following:

Lemma 4.2. *For all $\eta \in \mathbb{N}^3$, $\partial_q^\eta\big(\sqrt{1+|q|^2}\big)$ is a (finite) sum of terms of the form*

$$P_l(q)\left(1+|q|^2\right)^{-\frac{k}{2}} \tag{4.2}$$

with $l - k = 1 - |\eta|$, where P_l is a polynomial (in the three variables q_1, q_2, q_3), of degree at most l.

Proof. The proof is by induction after $|\eta| = n \in \mathbb{N}$. For $n = 1$, for some $j \in \{1, 2, 3\}$,

$$\partial_q^\eta\big(\sqrt{1+|q|^2}\big) = \frac{\partial}{\partial q_j}\big(\sqrt{1+|q|^2}\big) = \frac{q_j}{\sqrt{1+|q|^2}}$$

which is of the form described in (4.2). This proves the induction basis.

Assume now, for some $n \in \mathbb{N}$, that for all $\eta \in \mathbb{N}^3$, $|\eta| = n$, the function $\partial_q^\eta\big(\sqrt{1+|q|^2}\big)$ has the form described in (4.2). Take $\gamma \in \mathbb{N}^3$, $|\gamma| = n+1$, then $\gamma = \eta + e_j$, with $|\eta| = n$ and e_j one of the vectors $(1,0,0), (0,1,0), (0,0,1)$, and so

$$\partial_q^\gamma\big(\sqrt{1+|q|^2}\,\big) = \frac{\partial}{\partial q_j}\Big(\partial_q^\eta\big(\sqrt{1+|q|^2}\big)\Big).$$

By the induction hypothesis, this is a (finite) sum of terms of the forms

$$\begin{aligned}\frac{\partial}{\partial q_j}\left(P_l(q)\big(1+|q|^2\big)^{-\frac{k}{2}}\right) &= \left(\frac{\partial P_l}{\partial q_j}(q)\right)\left(\big(1+|q|^2\big)^{-\frac{k}{2}}\right)\\ &\quad + \big((-k)q_jP_l(q)\big)\big(1+|q|^2\big)^{-\frac{k+2}{2}} \qquad (4.3)\end{aligned}$$

with $l - k = 1 - n$. Rests to note that by the induction hypothesis $\frac{\partial}{\partial q_j}(P_l(q))$ is a polynomial of degree at most $l-1$ and $-kq_jP_l(q)$ one of degree at most $l+1$. Since $(l-1)-k = 1-(n+1)$ and $(l+1)-(k+2) = l-k-1 = 1-(n+1)$ by the induction hypothesis, the two terms in (4.3) are of the form described in (4.2), and the lemma now follows by induction. $\square$

Now, given a polynomial $P_l(q)$ of degree at most l, there exists a constant, $C = C(P_l)$, such that

$$|P_l(q)| \le C\left(1+|q|^l\right) \qquad \text{for all } q \in \mathbb{R}^3.$$

This means, by Lemma 4.2, since $k \ge l$, that

$$\left|P_l(q)\big(1+|q|^2\big)^{-\frac{k}{2}}\right| \le \left|P_l(q)\big(1+|q|^2\big)^{-\frac{l}{2}}\right| \le \frac{C(1+|q|^l)}{(1+|q|^2)^{\frac{l}{2}}} \le C,$$

with the same constant C as above, and so for all $\eta \in \mathbb{N}^3$ there exists a constant $C = C(\eta)$ such that

$$\left|\partial_q^\eta\big(\sqrt{1+|q|^2}\,\big)\right| \le C(\eta) \qquad \text{for all } q \in \mathbb{R}^3.$$

Since $a_\alpha + b \ge c$, this gives us (see (4.1)) , with $g(q) = \sqrt{1+q^2}$, that for $\eta \in \mathbb{N}^3$, $|\eta| \ge 2$,

$$\begin{aligned}\big|\partial_p^\eta a_\alpha(x,p)\big| &= \left|\partial_p^\eta\big(\sqrt{\alpha^{-1}p^2+\alpha^{-2}}\,\big)\right|\\ &= \big|\alpha^{-1+|\eta|/2}\big(\partial_q^\eta g\big)(\sqrt{\alpha}p)\big| \le C\left(a_\alpha(x,p)+b\right) \qquad (4.4)\end{aligned}$$

with a constant C independent of $\alpha \in]0,\alpha_0]$ (only depending on η, c and α_0). The reason we cannot use this for $|\eta| = 1$ is because of the α-scaling of things, see (4.1).

All in all, this means that for all $\gamma, \eta \in \mathbb{N}^3$ there exists a constant $C = C(\eta, \gamma, \alpha_0, b, c, V)$ such that

$$|\partial_p^\eta\partial_x^\gamma a_\alpha(x,p)| \le C\left(a_\alpha(x,p)+b\right)$$

for all $(x,p) \in \mathbb{R}_x^3 \times \mathbb{R}_p^3$, with C independent of $\alpha \in]0,\alpha_0]$. This finally proves that a_α is a symbol of weight $a_\alpha + b$, uniformly in $\alpha \in]0,\alpha_0]$. $\square$

One of the implications of this is that the following theorem holds (see Theorem A.10 in appendix A):

Theorem 4.3. *Let the operator H be the quantisation of the symbol a_α by $p \to -i\beta\nabla$ and let, for some $E, R > 0$, Θ be the quantisation of $\theta \in C_0^\infty(B_x(E) \times B_p(R))$. Then, for any $g \in C_0^\infty(\mathbb{R}^3)$, we have, uniformly in $\alpha \in]0, \alpha_0]$, that*

$$\operatorname{Tr}\{\Theta\, g(H)\} = (2\pi\beta)^{-3} \int \theta(x,p)\, g(a_\alpha(x,p))\, d^3x\, d^3p + \mathcal{O}(\beta^{-1}).$$

Lastly, we treat the so-called 'non-critical condition'; this will not be needed until later, but fits best here:

Lemma 4.4. *Assume that $a_\alpha(x,p) = \lambda$ and that*

$$|\lambda - V(x)| + |\nabla V(x)|^2 \geq \delta > 0.$$

Then

$$|\nabla a_\alpha(x,p)|^2 \geq \min\{\delta, \alpha_0^{-1}/2\}.$$

Proof. Note that $|\lambda - V(x)| = \sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1}$. Also,

$$|\nabla a_\alpha(x,p)|^2 = \frac{p^2}{\alpha p^2 + 1} + |\nabla V(x)|^2.$$

Now, for $\alpha p^2 \leq 1$, we have that

$$\frac{p^2}{\alpha p^2 + 1} \geq \frac{p^2}{2} \geq \frac{p^2}{\sqrt{\alpha p^2 + 1} + 1} = \sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1}$$

and so

$$|\nabla a_\alpha(x,p)|^2 \geq |\lambda - V(x)| + |\nabla V(x)|^2 \geq \delta.$$

For $\alpha p^2 \geq 1$ on the other hand,

$$|\nabla a_\alpha(x,p)|^2 \geq \frac{p^2}{\alpha p^2 + 1} \geq \frac{1}{2\alpha} \geq \frac{1}{2\alpha_0}.$$

This proves the lemma. $\square$

5. The Model Problem

We are ready to treat the 'model problem', namely with an 'abstract' operator A, in a ball with fixed radius, with a non-critical condition. By the method of Multi-scale Analysis, we will in the following section prove the same result without the non-critical condition (see (5.7)), for more specific functions g, and more general domains D.

The result will be build on the general semi-classical results in appendix A. The idea is to take advantage of the specific nature of the operator in question, expressed by the results in appendix B.

Throughout this section,

$$H = H(\beta, \alpha, V) = H_0 + V \quad , \quad H_0 = \sqrt{-\alpha^{-1}\beta^2\Delta + \alpha^{-2}} - \alpha^{-1},$$

$$a_\alpha(x,p) = \sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1} + V(x) \quad , \quad (x,p) \in \mathbb{R}^3_x \times \mathbb{R}^3_p,$$

with $V \in C_0^\infty(\mathbb{R}^3)$, and $\alpha \in]0, \alpha_0]$ and $\beta \in]0, \beta_0]$ for some fixed numbers α_0 and β_0. Since $H_0 \geq 0$, this means that $H \geq -\|V\|_\infty$. We will not here be needing the exact dependencies on this lower bound as computed in appendix B (there denoted M), nor the exact dependence on the radius of the ball on which we study the problem (denoted ρ in appendix B; here, this will be denoted E and will be fixed throughout). The reason for this is that the exact dependence on these (and other parameters) for the general problem will follow from the Multi-scale Analysis performed in the following section. One note on the dependence of the appearing cut-off function ψ: all estimates in section B require $|\psi| \leq 1$ (in section B, ψ is called χ); the estimates for general functions follow by normalizing.

About the abstract operator A we shall assume that it agrees with H on the open set $D \subset \mathbb{R}^3$ in the following sense:

Assumption 5.1.
A is selfadjoint in $L^2(\mathbb{R}^3)$, semi-bounded from below and for any $\zeta \in C_0^\infty(D)$ the following holds:

(1) $\forall u \in \mathcal{D}[A]$ we have $u\zeta \in \mathcal{D}[A]$. $\exists\, \zeta_1 \in C_0^\infty(D)$ (depending on ζ) such that $\zeta_1\zeta = \zeta$ and

$$A[u, \zeta v] = A[\zeta_1 u, \zeta v] + \big(B\, u, v\big) \quad \forall u, v \in \mathcal{D}[A],$$

with an operator B satisfying

$$\|B\|_1 \leq C_{N,D,\zeta_1} \left(\sqrt{\alpha}\beta\right)^N \qquad \text{for all } N \in \mathbb{N}. \tag{5.1}$$

If D is a ball of radius $\rho \geq \rho_0$ for some $\rho_0 > 0$ fixed, then

$$\|B\|_1 \leq C_{N,\zeta_1} \left(\frac{\sqrt{\alpha}\beta}{\rho}\right)^N \qquad \text{for all } N \in \mathbb{N}. \tag{5.2}$$

(2) $\exists\, V \in C_0^\infty(\mathbb{R}^3)$, real valued, such that, with $H = H_0 + V$, $v \in \mathcal{D}[A], u \in \mathcal{D}[H]$ we have $\zeta u \in \mathcal{D}[A], \zeta v \in \mathcal{D}[H]$ and

$$A[\zeta u, \zeta v] = H[\zeta u, \zeta v]$$

and

$$A\psi = H\psi \qquad \text{for all } \psi \in C_0^\infty(D). \tag{5.3}$$

(3) The operator A satisfies the lower bound $A \geq -\alpha^{-1}$.

Here, $\mathcal{D}[A]$ is the form domain of the operator A.

Remark 5.2. In particular, the operator A satisfies Assumption B.1 in appendix B; this means that all of the results in that appendix are at our disposition.

Let us define the class of functions g that we will be dealing with in this section (see definition A.11 in appendix A):

Definition 5.3. A function $g \in C^\infty(\mathbb{R} \setminus \{0\})$ is said to belong to the class $C^{\infty,s}(\mathbb{R})$ for $s \in [0,1]$ if:

(1) $g \in C(\mathbb{R})$, $s > 0$.
(2) For some $r > 0$ and some C:

$$\begin{aligned} g(\lambda) &= 0, && \lambda \geq C \\ |\partial_\lambda^m g(\lambda)| &\leq C_m |\lambda|^r, && \lambda \leq -C, \quad \forall m \geq 0. \end{aligned}$$

(3) For $|\lambda| \leq C$, $\lambda \neq 0$, and $m \geq 0$:

$$\begin{aligned} |\partial_\lambda^m g(\lambda)| &\leq C_m |\lambda|^{s-m}, && 0 < s < 1 \\ |\partial_\lambda^m g(\lambda)| &\leq C_m, && s = 0, 1. \end{aligned}$$

A function g is said to belong to $C_0^{\infty,s}(\mathbb{R})$, $s \in [0,1]$, if g is of compact support and $g \in C^{\infty,s}(\mathbb{R})$.

The main result of this section will be the following:

Theorem 5.4. *Let $\psi \in C_0^\infty(B(E/2))$ and $g \in C^{\infty,s}(\mathbb{R})$, $s \in [0,1]$. Suppose that the operator A satisfies Assumption 5.1 with $D = B(4E)$ and a potential $V \in C_0^\infty(\mathbb{R}^3)$, and that this potential satisfies*

$$|V(x)| + |\partial V(x)|^2 \geq c > 0, \qquad \forall x \in B(2E) \tag{5.4}$$

for some number c. Then

$$\begin{aligned} \mathrm{Tr}\{\psi\, g(A)\} = \frac{1}{(2\pi\beta)^3} \int \psi(x)\, g(a_\alpha(x,p))\, d^3x\, d^3p \\ + \mathcal{O}(\beta^{s-2}) + \mathcal{O}(\alpha^{-2}\beta^N) \quad , \quad \text{for all } N \in \mathbb{N}. \end{aligned} \tag{5.5}$$

The remainder estimate is uniform in V and ψ as long as these satisfy

$$|\partial^m V(x)| \leq C_m, \qquad |\partial^m \psi(x)| \leq C_m, \quad \forall m \in \mathbb{N}^3. \tag{5.6}$$

(That is, the remainders in the estimate (5.5) depend on the constants C_m's in (5.6), on g, α_0 and β_0, and on E).

Remark 5.5. For such general g, this is the best result we will prove; for the functions (here, $s \in [0,1]$)

$$g_s(\lambda) = \begin{cases} |\lambda|^s, & \lambda < 0 \\ 0, & \lambda \geq 0 \end{cases}$$

(which are all in $C^{\infty,s}$) we will in the next section remove the non-critical condition (5.4) by the Multi-scale Analysis; the possibility of this is due to the fact that for these functions g_s everything scales exactly as needed. We will also extend the result to more general domains than open balls.

Remark 5.6. In the theorem we can replace the condition (5.4) by

$$|V(x)| + |\partial V(x)|^2 + \beta \geq c > 0, \qquad \forall x \in B(2E), \tag{5.7}$$

since (5.4) implies that either

$$|V(x)| + |\partial V(x)|^2 \geq c/2 > 0, \qquad \forall x \in B(2E),$$

in which case the result follows from the theorem (with different constants C and C_N), or $\beta \geq c/2$. In this case, since by Lemma B.16

$$\|\psi g(A)\|_1 \leq C\, \alpha^{-3/2}\beta^{-3}$$

the trace $\mathrm{Tr}\{\psi\, g(A)\}$ is bounded by $C'\,\alpha^{-3/2}$, uniformly in β. Since $g(\lambda) = 0$ for $\lambda \geq C$, we have that

$$g(a_\alpha(x,p)) = 0 \quad \text{ for } \quad |p| \geq 1 + (C + \|V\|_\infty)\sqrt{\alpha_0} \equiv D_0$$

since $\sqrt{y^2+1} - 1 \geq (\sqrt{2}-1)|p|$ for $|p| \geq 1$. This means that

$$\left|\frac{1}{(2\pi\beta)^3}\int \psi(x)\, g(a_\alpha(x,p))\, d^3\!x\, d^3\!p\right| \\ \leq C\,\beta^{-3}\mathrm{Vol}\big(\mathrm{supp}\,\psi\big)\,\|\psi\|_\infty \frac{4\pi}{3} D_0^3 \leq \tilde{C}$$

and so we can write $\mathrm{Tr}\{\psi\, g(A)\}$ in the form (5.5).

The idea of the proof is the following: First, we establish the asymptotics for the 'true' operator, H. This is done by first choosing a C_0^∞-function f, equal to 1 on the support of g, and use the semi-classical analysis from appendix A on $f(H)$. Also, we show that to all orders in β, we can, for $f \in C_0^\infty(\mathbb{R})$, remove the quantised operator $\Theta = \mathrm{op}_\beta^w\theta$, $\theta \in C_0^\infty\big(B_x(E) \times B_p(R)\big)$, in the asymptotic expansion

$$\mathrm{Tr}\{\Theta\, f(H)\} = \frac{1}{(2\pi\beta)^3}\int \theta(x,p)\, f(a_\alpha(x,p))\, d^3\!x\, d^3\!p + \mathcal{O}(\beta^{-1}), \tag{5.8}$$

(see Theorem 4.3) as long as we insert the multiplication operator $\psi(x)$ (to have $\psi f(H)$) and as long as R is chosen large enough. This is of course due to the fact that for $f \in C_0^\infty(\mathbb{R})$, $f(a_\alpha(x,p)) = 0$ for $|p|$ large enough (see above). To relate the asymptotics for the 'true' operator, H, to that of the 'abstract' one, A, we compare the propagators of the two operators and take advantage of the important fact that the operators agree on the set $C_0^\infty(B(3E))$. We then use that this set contains the image of a Fourier integral operator $G_\beta(t)$ (see (A.11)) that approximates both the propagator of H and that of A. Finally, to end the proof, we use the Tauberian argument from Proposition A.12 to remove the introduced C_0^∞-function f, and by splitting the function g in sums of functions with different properties, we get the result for the general class of functions, $C^{\infty,s}(\mathbb{R})$.

Throughout this section, we shall use the notation

$$A_1(\beta) \sim A_2(\beta)$$

when, for the two families of operators, $A_1(\beta)$ and $A_2(\beta)$, we have

$$\|A_1(\beta) - A_2(\beta)\|_1 \leq C_N \alpha^{-3/2}\beta^N, \quad \forall N \in \mathbb{N},$$

with a constant only depending on N and the fixed numbers α_0, β_0 and E.

First we wish to prove that the localisation in phase-space (by the operator $\Theta = \mathrm{op}^w_\beta \theta$) can be removed, as long as we have a localisation in configuration space (by the function ψ) and a function g with compact support.

Lemma 5.7. *Let $\psi \in C_0^\infty(B(E/2))$, $g \in C_0^\infty(\mathbb{R})$, and let the function $\theta \in C_0^\infty\big(B_x(E) \times B_p(R)\big)$ satisfy*

$$\theta(x,p) = 1 \text{ on } B_x(5E/6) \times B_p(R/2),$$

with

$$R \geq 2\Big(1 + \frac{\big(\max_x g(x) + 2 + \|V\|_\infty\big)\sqrt{\alpha_0}}{\sqrt{2}-1}\Big). \tag{5.9}$$

Then, with $\Theta = \mathrm{op}^w_\beta \theta$ the quantisation of the symbol θ, we have

$$\|\psi g(H)(I - \Theta)\|_1 \leq C_N \alpha^{-3/2}\beta^N \quad \forall N > 0. \tag{5.10}$$

The constant depends on g and θ, and on α_0, β_0 and E.

Proof. Let $\psi_1 \in C_0^\infty(B(3E/4))$ be a function such that $\psi_1(x) = 1$, $x \in B(5E/8)$. This means that, with $\phi = 1 - \psi_1$,

$$\mathrm{dist}\{\mathrm{supp}\,\psi, \mathrm{supp}\,\phi\} \geq E/8$$

and so the pair of functions ψ, ϕ satisfies the condition (B.6) of Theorem B.19, so

$$\|\psi g(H)\phi\|_1 \leq C_N \alpha^{-3/2}\beta^N \quad \forall N > 0. \tag{5.11}$$

Note that since $g \in C_0^\infty(\mathbb{R})$, the condition (B.79) is trivially satisfied. Choose also a function $f \in C_0^\infty(\mathbb{R})$ such that $f \equiv 1$ on $\mathrm{supp}\, g$; more explicitely, such that

$$f(x) = \begin{cases} 0 & x \leq (\min_x g(x)) - 2 \\ 1 & x \in [(\min_x g(x)) - 1, (\max_x g(x)) + 1] \\ 0 & x \geq (\max_x g(x)) + 2. \end{cases}$$

In this way,

$$\mathrm{dist}\{\mathrm{supp}\,(1-f), \mathrm{supp}\, g\} \geq 1 > 0.$$

Since $fg = g$ this means that (remember that $\psi_1 + \phi = 1$)

$$\begin{aligned} &\|\psi g(H) - \psi g(H)\psi_1 f(H)\|_1 \\ &\qquad = \|\psi g(H)(\psi_1 + \phi) f(H) - \psi g(H)\psi_1 f(H)\|_1 \\ &\qquad = \|\psi g(H)\phi f(H)\|_1 \leq C_N \alpha^{-3/2}\beta^N \quad \forall N > 0, \end{aligned}$$

since, by the spectral theorem, $f(H)$ is bounded, independently of α and β, and so

$$\psi g(H) \sim \psi g(H)\psi_1 f(H).$$

Now, since, by Lemma B.10 (remember that $\alpha \in]0, \alpha_0]$)

$$\|\psi g(H)\|_1 \leq C\,\alpha^{-3/2}\beta^{-3},$$

it suffices to check that for R as in (5.9),

$$\|\psi_1 f(H)(I - \Theta)\| \leq C_N \beta^N \quad \forall N > 0. \tag{5.12}$$

(Note, that this is in operator norm, not in the trace norm; the introduction of ψ_1 and f served to get rid of the question of trace norm and pass the problem to one of operator norm, the price being the negative power of α). Next we have, by Lemma 4.1, that the symbol

$$a_\alpha(x,p) = \sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1} + V(x)$$

satisfies

1) $\exists\, b, c > 0 : a_\alpha + b \geq c$
2) $a_\alpha + b$ is a weight
3) a_α is a symbol of weight $a_\alpha + b$.

All of this, uniformly in $\alpha \in]0, \alpha_0]$. This means (see Theorem A.6) that the operator H is β-admissible, uniformly in α, that is, since $f \in C_0^\infty(\mathbb{R})$, we have the representation

$$f(H) = \sum_{j=0}^{N} \beta^j \mathrm{op}_h^w a_{\alpha,f,j} + \beta^{N+1} R_{g,N+1}(\beta), \tag{5.13}$$

where the $a_{\alpha,f,j}$'s are given by

$$\begin{aligned}
a_{\alpha,f,0}(x,p) &= f(a_\alpha(x,p)),\\
a_{\alpha,f,1}(x,p) &= 0,\\
a_{\alpha,f,j}(x,p) &= \sum_{k=1}^{2j-1} \frac{(-1)^k}{k!}\, d_{j,k}\, \partial_\lambda^k f(a_\alpha(x,p)) \quad , \quad j \geq 2.
\end{aligned}$$

(the coefficients $d_{j,k}$ are universal polynomials of $\partial_x^{m_1}\partial_p^{m_2} a_\alpha$, $m_1 + m_2 \leq j$) and where $\|R_{f,N+1}(\beta)\| \leq C_N$, independently of α and β. This means, since the operator $I - \Theta$ is bounded, also independently of α and β, that the bound (5.12) is fulfilled for the remainder

$$\beta^{N+1} R_{g,N+1}(\beta)(I - \Theta).$$

To prove the estimate (5.12) for the other terms, we observe that this amounts to proving, that the product of three operators with the symbols

$$\psi_1(x), \quad \partial_\lambda^m f(a_\alpha(x,p)), \quad 1 - \theta(x,p), \quad m = 0, 1, \ldots$$

satisfies the estimate (5.12). Now, $f \in C_0^\infty(\mathbb{R})$, and so

$$\operatorname{supp} f(a_\alpha(\cdot,\cdot)) \subset \{(x,p) \mid |p| \leq C\}$$

with

$$C = \Big(1 + \frac{\big(\max_x g(x) + 2 + \|V\|_\infty\big)\sqrt{\alpha_0}}{\sqrt{2}-1}\Big). \tag{5.14}$$

To see this, note that

$$\sqrt{y^2+1} - 1 \geq \begin{cases} c\,y, & y \geq 1 \\ c\,y^2, & y \in [0,1] \end{cases}$$

with $c = \sqrt{2}-1$. Note, that C above is independent of α. That is,

$$\operatorname{supp} \psi_1 \cap \operatorname{supp} f(a_\alpha(\cdot,\cdot)) \subset \{(x,p) \mid |x| \leq 3E/4, |p| \leq C\}.$$

Now, since

$$\theta(x,p) = 1 \text{ for } (x,p) \in B_x(5E/6) \times B_p(R/2)$$

for some $R \geq 2\,C$ (see (5.9)), we have that

$$\operatorname{supp} \psi_1 \cap \operatorname{supp} \partial_\lambda^m f(a_\alpha(\cdot,\cdot)) \cap \operatorname{supp}(1-\theta) = \emptyset.$$

From Lemma A.5 in appendix A now follows, that

$$\|\psi_1 \operatorname{op}_\beta^w a_{\alpha,f,n}\,(I - \Theta)\| \leq C_N \beta^N, \quad \forall N > 0.$$

This proves the lemma. $\square$

This result will allow us to replace the quantisation $\Theta = \operatorname{op}_\beta^w \theta$ of θ, the cut-off in phase-space, with the multiplication operator ψ, a cut-off in configuration space only, in the following sense:

Lemma 5.8. *Let $\psi \in C_0^\infty(B(E/2))$.*

(1) If $g \in C_0^\infty(\mathbb{R})$, then

$$\operatorname{Tr}\{\psi\, g(H)\} = \frac{1}{(2\pi\beta)^3} \int \psi(x) g(a_\alpha(x,p))\, d^3x\, d^3p + \mathcal{O}(\beta^{-1}) + \mathcal{O}(\alpha^{-3/2}\beta^N) \text{ for all } N > 0. \tag{5.15}$$

(2) Suppose that for some λ, with $|\lambda| \leq \lambda_0$ for some fixed λ_0, the 'non-critical' condition

$$|V(x) - \lambda| + |\partial V(x)|^2 \geq c > 0 \qquad \forall x \in B(2E) \tag{5.16}$$

is satisfied. Then

$$\|\psi f(H) \chi_\beta(H-\lambda)\|_1 \leq C\,\beta^{-3} + C_N \alpha^{-3/2}\beta^N \text{ for all } N > 0. \tag{5.17}$$

The constants C and C_N are uniform in $|\lambda| \leq \lambda_0$. Here,

$$\chi_\beta(\tau) = \frac{1}{\beta}\chi_1\left(\frac{\tau}{\beta}\right)$$

with the function χ_1 being the Fourier transform of a function $\hat{\chi} \in C_0^\infty(-T,T)$, satisfying

$$\begin{aligned} \hat{\chi}(t) &= \hat{\chi}(-t) \in \mathbb{R} \qquad \forall t, \\ \hat{\chi}(t) &= 1 \quad , \quad |t| \le T/2. \end{aligned}$$

Additionally, we have that $\chi_1 \ge 0$ and that there exists a $T_1 \in]0,T[$, such that $\chi_1(\tau) \ge c > 0$ for $|\tau| \le T_1$ (see (A.13) for further details).
(3) Let g be a compactly supported function in $L^1(\mathbb{R})$ and let the 'non-critical' condition (5.16) above be fulfilled for all $\lambda \in \operatorname{supp} g$. Then

$$\begin{aligned} &\operatorname{Tr}\{\psi\, f(H) g^{(\beta)}(H)\} \\ &\quad = \frac{1}{(2\pi\beta)^3} \int \psi(x) g(a_\alpha(x,p))\, d^3x\, d^3p \\ &\qquad + \mathcal{O}(\beta^{-1}) + \mathcal{O}(\alpha^{-3/2}\beta^N) \text{ for all } N > 0. \end{aligned} \tag{5.18}$$

Here,

$$g^{(\beta)}(\tau) = \int g(\tau - \nu)\chi_\beta(\nu)\, d\nu = \int g(\nu)\chi_\beta(\tau - \nu)\, d\nu$$

with χ_β as above.

Remark 5.9. Note that in the last result, the trace of the operator $\psi f(H) g^{(\beta)}(H)$ is related to the semi-classical integral of the function g itself. Later, by the Tauberian argument in Proposition A.12, this will be related to the trace of $\psi g(H)$.

Proof. The ingredients are the semi-classical results from appendix A and the lemma just proven.

We start by proving (5.18). Without loss of generality, assume that $g(\lambda)$ and $\psi(x)$ are real-valued (for complex-valued, write as $\psi = \operatorname{Re}\psi + i\operatorname{Im}\psi$ and expand the product). Let θ be the symbol from Lemma 5.7, so that the same lemma (used on the function f) gives, that

$$\psi f(H) g^{(\beta)}(H) \sim \psi f(H)\, \Theta\, g^{(\beta)}(H)$$

since, by (A.16) and the spectral theorem, $\|g^{(\beta)}(H)\| \le C\,\beta^{-1}$, independently of α. The idea is now, by aid of the expansion (A.9) and the product formula (A.5) in appendix A, to compute the first couple of terms in the expansion in powers of β of the symbol of the operator $\psi\, f(H)\, \Theta$. To this end, recall (see (5.13)), that

$$f(H) = \operatorname{op}^w_\beta f(a_\alpha) + \beta^2 R_{f,2}(\beta)$$

since $a_{\alpha,f,1} \equiv 0$. This means, that

$$\psi\, f(H)\, \Theta = \psi\, \operatorname{op}^w_\beta f(a_\alpha)\, \Theta + \beta^2 \psi\, R_{f,2}(\beta)\, \Theta$$

with

$$\|\beta^2 \psi R_{f,2}(\beta)\,\Theta\|_1 \leq \beta^2 \|\psi\|\,\|R_{f,2}(\beta)\|\,\|\Theta\|_1 \leq C\,\beta^{-1}$$

since $\|R_{f,2}(\beta)\| \leq C$, uniformly in α and β, and $\|\Theta\|_1 \leq C\,\beta^{-3}$ by (A.4), uniformly in α, as $\theta \in C_0^\infty(\mathbb{R}^3_x \times \mathbb{R}^3_p)$. Next, by the formula (A.5) in appendix A

$$\psi\,\mathrm{op}^w_\beta f(a_\alpha) = \big(\mathrm{op}^w_\beta \psi\big)\big(\mathrm{op}^w_\beta f(a_\alpha)\big) = \mathrm{op}^w_\beta q$$

with

$$\begin{aligned} q(x,p) &= \psi(x)\, f(a_\alpha(x,p)) \\ &+ \sum_{|m_1|+|m_2|=1} (-i)(-1)^{|m_2|}\frac{i\beta}{4}\big(\partial_p^{m_1}\,\partial_x^{m_2}\psi(x)\,\partial_p^{m_2}\partial_x^{m_1} f(a_\alpha(x,p))\big) \\ &\qquad + \beta^2 r_2(x,p;\beta), \end{aligned}$$

where the operator $R_2(\beta) = \mathrm{op}^w_\beta r_2$ is bounded uniformly in $f(a_\alpha)$ and ψ; that is, $\|R_2(\beta)\| \leq C_2$, independently of β and α (the constant C_2 depends on the constants in the weight estimates (A.1) of $a_{\alpha,f,0} = f(a_\alpha)$ and ψ, and these are independent of α.) Using (A.5) again, we get that

$$\psi\,\mathrm{op}^w_\beta f(a_\alpha)\,\Theta = \big(\mathrm{op}^w_\beta q\big)\,\big(\mathrm{op}^w_\beta \theta\big) = \mathrm{op}^w_\beta s$$

with

$$\begin{aligned} s(x,p) &= q(x,p)\,\theta(x,p) \\ &+ \sum_{|\tilde m_1|+|\tilde m_2|=1} (-i)(-1)^{|\tilde m_2|}\frac{i\beta}{4}\big(\partial_p^{\tilde m_1}\partial_x^{\tilde m_2} q(x,p)\big)\,\big(\partial_p^{\tilde m_2}\partial_x^{\tilde m_1}\theta(x,p)\big) \\ &\qquad + \beta^2 \tilde r_2(x,p;\beta) \\ &= \psi(x)\, f(a_\alpha(x,p))\,\theta(x,p) + i\beta\mathcal{A}(x,p) + \beta^2\mathcal{B}(x,p) + i\beta^3\mathcal{C}(x,p). \end{aligned}$$

Here,

$$\begin{aligned} &\mathcal{A}(x,p) \\ &\quad = \sum_{|m_1|+|m_2|=1} (-i)(-1)^{|m_2|}\frac{1}{4}\big(\partial_p^{m_1}\,\partial_x^{m_2}\psi(x)\,\partial_p^{m_2}\partial_x^{m_1} f(a_\alpha(x,p))\big)\,\theta(x,p) \\ &+ \sum_{|\tilde m_1|+|\tilde m_2|=1} (-i)(-1)^{|\tilde m_2|}\frac{1}{4}\Big(\partial_p^{\tilde m_1}\partial_x^{\tilde m_2}\big(\psi(x)\, f(a_\alpha(x,p))\big)\Big)\,\Big(\partial_p^{\tilde m_2}\partial_x^{\tilde m_1}\theta(x,p)\Big) \\ &\qquad \in \mathbb{R} \end{aligned}$$

and

$$\begin{aligned} \mathcal{B}(x,p) &= \tilde r_2(x,p;\beta) + r_2(x,p;\beta)\,\theta(x,p) \\ &- \sum_{\substack{|m_1|+|m_2|=1 \\ |\tilde m_1|+|\tilde m_2|=1}} \frac{(-1)^{|\tilde m_2|+|m_2|}}{16}\Big(\partial_p^{\tilde m_1}\partial_x^{\tilde m_2}\big(\partial_p^{m_1}\partial_x^{m_2}\psi(x)\,\partial_p^{m_2}\partial_x^{m_1} f(a_\alpha(x,p))\big)\Big) \\ &\qquad \times \big(\partial_p^{\tilde m_2}\partial_x^{\tilde m_1}\theta(x,p)\big) \end{aligned}$$

and

$$\mathcal{C}(x,p) = \sum_{|\tilde{m}_1|+|\tilde{m}_2|=1} (-i)(-1)^{|\tilde{m}_2|}\frac{1}{4}\big(\partial_p^{\tilde{m}_1}\partial_x^{\tilde{m}_2} r_2(x,p;\beta)\big)\,\big(\partial_p^{\tilde{m}_2}\partial_x^{\tilde{m}_1}\theta(x,p)\big).$$

By (A.4) in Proposition A.4 (since θ is of compact support),

$$\|\mathrm{op}_\beta^w\big(\partial_p^{\tilde{m}_2}\partial_x^{\tilde{m}_1}\theta\big)\|_1 \le C\,\beta^{-3}$$
$$\|\mathrm{op}_\beta^w\theta\|_1 \le C\,\beta^{-3}$$

and as mentioned earlier,

$$\|\mathrm{op}_\beta^w r_2\| = \|R_2(\beta)\| \le C.$$

Since θ is of compact support, the rest $\mathrm{op}_\beta^w\tilde{r}_2 = \tilde{R}_2(\beta)$ by (A.6) satisfies

$$\|\mathrm{op}_\beta^w\tilde{r}_2\|_1 = \|\tilde{R}_2(\beta)\|_1 \le C\,\beta^{-3}.$$

In this way,

$$\psi\,f(H)\,\Theta = \mathrm{op}_\beta^w\big(\psi\,f(a_\alpha)\,\theta\big) + i\beta\mathrm{op}_\beta^w(\mathcal{A}) + \beta^2\mathrm{op}_\beta^w(\mathcal{E})$$

where

$$\|\mathrm{op}_\beta^w(\mathcal{E})\|_1 \le C\,\beta^{-3}$$

and $\mathrm{Im}\,\mathcal{A} \equiv 0$. That is,

$$\|\psi\,f(H)\,\Theta - \mathrm{op}_\beta^w(\psi\,f(a_\alpha)\,\theta) - i\beta\,\mathrm{op}_\beta^w(\mathcal{A})\|_1 \le C\,\beta^{-1}.$$

This means that

$$\begin{aligned}
&\mathrm{Tr}\{\psi\,f(H)\,g^{(\beta)}(H)\}\\
&= \mathrm{Tr}\{\psi\,f(H)\,\Theta\,g^{(\beta)}(H)\} + \mathcal{O}(\alpha^{-3/2}\beta^N), \quad \forall N>0\\
&= \mathrm{Tr}\{\tilde{\theta}\,g^{(\beta)}(H)\} + i\beta\,\mathrm{Tr}\{\mathrm{op}_\beta^w(\mathcal{A})\,g^{(\beta)}(H)\}\\
&\qquad + \mathcal{O}(\beta^{-1}) + \mathcal{O}(\alpha^{-3/2}\beta^N), \quad \forall N>0
\end{aligned} \tag{5.19}$$

with

$$\tilde{\theta} = \psi\,f(a_\alpha)\,\theta, \quad \mathrm{supp}\,\tilde{\theta} \subset \mathrm{supp}\,\theta,$$

since, again, $\|g^{(\beta)}(H)\| \le C\,\beta^{-1}$, by the spectral theorem and (A.16). Now, note that since all symbols and g are real-valued, and the operator H is self-adjoint, then the involved operators are self-adjoint and so all traces in the above formula are real. This means that

$$i\beta\,\mathrm{Tr}\{\mathrm{op}_\beta^w(A)\,g^{(\beta)}(H)\} = \mathcal{O}(\beta^{-1}) + \mathcal{O}(\alpha^{-3/2}\beta^N), \quad \forall N>0.$$

By Lemma 4.4, we have that

$$a_\alpha(x,p) = \lambda \text{ and } |V(x)-\lambda| + |\partial V(x)|^2 \ge \delta > 0$$

implies that

$$|\nabla a_\alpha(x,p)|^2 \ge \min\{\delta, {\alpha_0}^{-1}/2\},$$

so that the non-critical condition (see (A.17) in Assumption A.9) on the gradient is satisfied on the 'energy shell' of energy λ for all $\lambda \in \mathrm{supp}\,g$.

Furthermore, $\tilde\theta \in C_0^\infty(\mathbb{R}^3_x \times \mathbb{R}^3_p)$ and $\operatorname{supp}\tilde\theta \subset B_x(E) \times B_p(R)$, so (3) in Proposition A.10 gives us the asymptotics

$$\operatorname{Tr}\{\tilde\theta\, g^{(\beta)}(H)\} = \frac{1}{(2\pi\beta)^3}\int \tilde\theta(x,p)\, g(a_\alpha(x,p))\, d^3\!x\, d^3\!p + \mathcal{O}(\beta^{-1}). \tag{5.20}$$

Notice, that this is uniformly in α. Now, as before,

$$\operatorname{supp} g(a_\alpha(\cdot,\cdot)) \subset \{(x,p) \mid |p| \le C\}$$

with C as in (5.14), and so, by (5.9), we get that

$$\theta(x,p) = 1 \text{ for } |p| \le C \text{ and } x \in \operatorname{supp}\psi.$$

This means that

$$\psi(x)\theta(x,p)g(a_\alpha(x,p)) = \psi(x)g(a_\alpha(x,p)) \quad \forall (x,p),$$

so that, since $fg = g$,

$$\begin{aligned}\tilde\theta(x,p)g(a_\alpha(x,p)) &= \psi(x)\theta(x,p)f(a_\alpha(x,p))g(a_\alpha(x,p))\\ &= \psi(x)g(a_\alpha(x,p)) \qquad \forall (x,p).\end{aligned}$$

This means, by (5.19) and (5.20), that

$$\begin{aligned}\operatorname{Tr}\{\psi\, f(H)g^{(\beta)}(H)\} = \frac{1}{(2\pi\beta)^3}&\int \psi(x)\, g(a_\alpha(x,p))\, d^3\!x\, d^3\!p\\ &+ \mathcal{O}(\beta^{-1}) + \mathcal{O}(\alpha^{-3/2}\beta^N) \quad \text{for all } N > 0.\end{aligned}$$

This proves (5.18).

To prove (5.15), notice that by Lemma 5.7, $\psi\, g(H) \sim \psi\, g(H)\,\Theta$. Next, as in the proof above, we can find a sub-principal symbol $\tilde{\mathcal{A}}$ for the operator $\psi\, g(H)\,\Theta$, such that $\operatorname{Im}\tilde{\mathcal{A}} \equiv 0$ and such that the we have the estimate

$$\|\psi\, g(H)\,\Theta - \operatorname{op}^w_\beta(\psi\, g(a_\alpha)\,\theta) - i\beta\operatorname{op}^w_\beta(\tilde{\mathcal{A}})\|_1 \le C\,\beta^{-1}.$$

As before, by choosing the same R, we can assure that

$$\begin{aligned}\tilde\theta(x,p)\, g(a_\alpha(x,p)) &= \psi(x)\, g(a_\alpha(x,p))\,\theta(x,p)\\ &= \psi(x)\, g(a_\alpha(x,p)) \quad \forall (x,p),\end{aligned}$$

and so this proves (5.15) by (1) in Proposition A.10 as above.

Finally, to prove (5.17), note that by the spectral theorem and (A.14), $\|\chi_\beta(H-\lambda)\| \le C\,\beta^{-1}$, and so

$$\psi f(H)\chi_\beta(H-\lambda) \sim \psi f(H)\,\Theta\,\chi_\beta(H-\lambda)$$

by Lemma 5.7, since $f \in C_0^\infty(\mathbb{R})$. Also, $\|\psi f(H)\| \le C$ by the spectral theorem, and so, by (3.1) and (2) in Proposition A.10, we get, that

$$\begin{aligned}&\|\psi\, f(H)\chi_\beta(H-\lambda)\|_1\\ &\qquad \le \|\psi\, f(H)\|\,\|\Theta\,\chi_\beta(H-\lambda)\|_1 + C\,\alpha^{-3/2}\beta^N \text{ for all } N > 0\\ &\qquad \le C\,\beta^{-3} + C_N\alpha^{-3/2}\beta^N \quad \text{for all } N > 0.\end{aligned}$$

This finishes the proof of the lemma. □

The next step will be to compare the propagators of (the time evolution of) the two operators H and A. This will be done by intermediary of the Fourier integral operator (FIO) $G_\beta(t)$, defined in (A.11), which will be shown to approximate both propagators.

Denote the propagators of H and A by $U_\beta(t;H)$ and $U_\beta(t;A)$, respectively. The result we are aiming at is the following:

Lemma 5.10. *Let the operator A satisfy Assumption 5.1 with $D = B(4E)$ and let $f \in C_0^\infty(\mathbb{R}^3)$. Then there exists a number $T_0 > 0$ such that for $|t| \leq T_0$ we have*

$$\|\psi\, f(H)\big(U_\beta(t;H) - U_\beta(t;A)\big)\|_1 \leq C_N \alpha^{-3/2}\beta^N, \qquad \text{for all } N > 0. \tag{5.21}$$

The constant C_N is uniform in ψ and V obeying the bounds (5.6) (see also formulation in Theorem 5.4).

Proof. As earlier mentioned, the idea is to approximate the two propagators by a Fourier integral operator. The second ingredient is Lemma 5.7. Since the symbol $a_\alpha(x,p)$ is smooth, we can use the techniques from appendix A. Let therefore θ be the symbol from Lemma 5.7 and let $G_\beta(t)$ denote the β-FIO with the kernel

$$\mathcal{G}(x,y,t) = \frac{1}{(2\pi\beta)^3}\int e^{\frac{i}{\beta}(S(x,p,t)-y\cdot p)} v(x,p,t;\beta)\, d^3p.$$

By Proposition A.8, there exists a number (a 'time') T_0 and smooth functions

$$S, v \in C^\infty\big(B_x(3E)\times B_\xi(3R)\times[-T_0,T_0]\big)$$

such that, defining the operator $G_\beta(t)$ as above with this choice of S and v,

$$\sup_{|t|\leq T_0} \| -i\beta\partial_t G_\beta(t) + HG_\beta(t)\| \leq C_N\beta^{N+1}. \tag{5.22}$$

Note, that T_0 and the C_N's are independent of $\alpha \in]0,\alpha_0]$.

Now, $G_\beta(t)$ acts into $C_0^\infty(B(3E))$, and so, since H and A agree on this set (see (1) in Assumption 5.1), we have, that

$$HG_\beta(t) = AG_\beta(t) \qquad \text{for all } t. \tag{5.23}$$

This and the estimate (5.22) is what will allow us to show, that $G_\beta(t)$ approximates not only the time-evolution (the propagator) $U_\beta(t;H)$ of H, but also $U_\beta(t;A)$, that of A. More explicitely, we will prove the following estimate:

$$\sup_{|t|\leq T_0} \|\Theta\big(U_\beta(t) - G_\beta(t)\big)\|_1 \leq C_N\beta^{N-3} \text{ for all } N\in\mathbb{N},\ \alpha\in]0,\alpha_0]. \tag{5.24}$$

Here, $U_\beta(t)$ denotes any of the two propagators, $U_\beta(t;H)$ or $U_\beta(t;A)$.

To prove this for $U_\beta(t;A)$, let

$$M_\beta(t) = -i\beta\partial_\beta G_\beta(t) + A\,G_\beta(t)$$

and remember the initial condition (A.12):

$$G_\beta(0) = \Phi$$

where $\Phi = \mathrm{op}^w_\beta \phi$, with a real valued function ϕ such that

$$\begin{aligned}
&\phi \in C_0^\infty\big(B_x(2E) \times B_p(2R)\big)\\
&\phi(x,p) = 1, \quad (x,p) \in B_x(3E/2) \times B_p(3R/2)
\end{aligned}$$

(in this way, the supports of θ and $1-\phi$ are disjoint). Now, the propagator $U_\beta(t;A)$ is defined as the solution to the evolution equation

$$-i\beta\partial_t U_\beta(t;A) + A\,U_\beta(t;A) = 0, \quad U_\beta(0;A) = I$$

and so the difference

$$E_\beta(t) = U_\beta(t;A) - G_\beta(t)$$

will satisfy

$$-i\beta\partial_t E_\beta(t) + A\,E_\beta(t) = -M_\beta(t), \quad E_\beta(0) = I - \Phi. \tag{5.25}$$

Integrating this equation, we get

$$E_\beta(t) = -\frac{i}{\beta}\int_0^t U_\beta(t-s;A) M_\beta(s)\,ds + (I - \Phi)$$

(check by differentiating and inserting in (5.25) above). This means, that

$$\sup_{|t|\le T_0} \|\Theta\,E_\beta(t)\|_1 \le \frac{T_0}{\beta}\,\|\Theta\|_1 \sup_{|t|\le T_0} \|M_\beta(t)\| + \|\Theta(I-\Phi)\|_1,$$

since $U_\beta(t;A)$ is unitary and so of norm less than or equal to one. As noted above, the supports of θ and $1-\phi$ are disjoint, and so the term $\|\Theta(I-\ \Phi)\|_1$ satisfy the estimate (5.24) by (A.8) in Lemma A.5. To estimate $\|M_\beta(t)\|$, we use the fact that (see (5.23))

$$H\,G_\beta(t) = A\,G_\beta(t) \qquad \text{for all } t$$

and the estimate (5.22). This gives us, that

$$\sup_{|t|\le T_0} \|M_\beta(t)\| = \sup_{|t|\le T_0} \|-i\beta\partial_\beta G_\beta(t) + H\,G_\beta(t)\|_1 \le C_N \beta^{N+1}.$$

Now, since $\Theta = \mathrm{op}^w_\beta \theta$ and $\theta \in C_0^\infty\big(B_x(E) \times B_p(R)\big)$, the estimate $\|\Theta\|_1 \le C\,\beta^{-3}$ from (A.4) in Proposition A.4 gives us that

$$\sup_{|t|\le T_0} \|\Theta\,\big(U_\beta(t;A) - G_\beta(t)\big)\|_1 = \sup_{|t|\le T_0} \|\Theta\,E_\beta(t)\|_1 \le C_N \beta^{N-3}.$$

This proves the estimate (5.24) for the propagator $U_\beta(t;A)$ of A; for that of $U_\beta(t;H)$, the proof goes as above, except that we can use (5.22) directly.

To prove the lemma, we write

$$\psi\, f(H)\big[U_\beta(t;H) - U_\beta(t;A)\big] = \psi\, f(H)(I-\Theta)\big[U_\beta(t;H) - U_\beta(t;A)\big] + \psi\, f(H)\,\Theta\,\big[U_\beta(t;H) - U_\beta(t;A)\big]$$

and so

$$\begin{aligned}\|\psi\, f(H)\big(U_\beta(t;H) - U_\beta(t;A)\big)\|_1 &\\ \leq \|\psi\, f(H)(I-\Theta)\|_1\, \|U_\beta(t;H) - U_\beta(t;A)\| &\\ + \|\psi\, f(H)\|\, \|\Theta\big(U_\beta(t;H) - U_\beta(t;A)\big)\|_1 &\\ \leq 2\|\psi\, f(H)(I-\Theta)\|_1 + C\,\|\Theta\,\big(U_\beta(t;H) - U_\beta(t;A)\big)\|_1 &\end{aligned}$$

since $U_\beta(t;H)$, resp. $U_\beta(t;A)$, are unitary, and $\|\psi f(H)\| \leq \|\psi\|_\infty \|f\|_\infty$ by the spectral theorem.

The estimate (5.21) for the first term now follows from Lemma 5.7, whereas for the second, it follows from applying the bound (5.24) twice, substracting and adding $G_\beta(t)$ (remember that $\alpha \in]0, \alpha_0]$). This proves the lemma. □

This result allows us to prove the estimates in Lemma 5.8 for the operator A:

Lemma 5.11. *Let A be as in Theorem 5.4 and let $\psi \in C_0^\infty(B(E/2))$.*

(1) If $g \in C_0^\infty(\mathbb{R})$, then

$$\mathrm{Tr}\{\psi\, g(A)\} = \frac{1}{(2\pi\beta)^3}\int \psi(x) g(a_\alpha(x,p))\, d^3x\, d^3p + \mathcal{O}(\beta^{-1}) + \mathcal{O}(\alpha^{-2}\beta^N) \quad \textit{for all } N > 0. \tag{5.26}$$

(2) Suppose that for some λ, with $|\lambda| \leq \lambda_0$ for some λ_0 fixed, the 'non-critical' condition

$$|V(x) - \lambda| + |\partial V(x)|^2 \geq c > 0 \qquad \forall x \in B(2E) \tag{5.27}$$

is satisfied. Then

$$\|\psi f(A)\chi_\beta(A-\lambda)\|_1 \leq C\,\beta^{-3} + C_N \alpha^{-2}\beta^N \quad \textit{for all } N > 0. \tag{5.28}$$

The constants C and C_N are uniform in $|\lambda| \leq \lambda_0$. (See Lemma 5.8 for the function χ_β.)

(3) Let $g \in L^1(\mathbb{R})$ be a compactly supported function and let the 'non-critical' condition (5.27) be fulfilled for all $\lambda \in \operatorname{supp} g$. Then

$$\mathrm{Tr}\{\psi\, f(A) g^{(\beta)}(A)\} = \frac{1}{(2\pi\beta)^3}\int \psi(x) g(a_\alpha(x,p))\, d^3x\, d^3p + \mathcal{O}(\beta^{-1}) + \mathcal{O}(\alpha^{-2}\beta^N) \quad \textit{for all } N > 0. \tag{5.29}$$

Here, as before,

$$a_\alpha(x,p) = \sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1} + V(x).$$

Proof. By Theorem B.18

$$\|\psi[g(H) - g(A)]\|_1 \le C_N \alpha^{-2}\beta^N \quad \text{for all } N > 0, \tag{5.30}$$

since $g \in C_0^\infty(\mathbb{R})$ (and therefore trivially satisfies the condition (B.72)) and so (5.26) follows from the analogue result (5.15) for the operator H (remember that $\alpha \in]0, \alpha_0]$).

Since $\|g^{(\beta)}(H)\| \le C\,\beta^{-1}$ and $\|\chi_\beta(A-\lambda)\| \le C\,\beta^{-1}$ by the spectral theorem (see (A.16) and (A.14)), the estimate (5.30) above (applied to $f \in C_0^\infty(\mathbb{R})$) gives that

$$\begin{aligned}\|\psi\, f(A)\chi_\beta(A-\lambda) - \psi\, f(H)\chi_\beta(A-\lambda)\|_1 \\ \le C_N\alpha^{-2}\beta^N \quad \text{for all } N > 0,\end{aligned}$$

and

$$\|\psi\, f(A)\, g^{(\beta)}(A) - \psi\, f(H)\, g^{(\beta)}(A)\|_1 \le C_N'\alpha^{-2}\beta^N \quad \text{for all } N > 0.$$

Next, by definition (see (A.13), (A.14) and (A.15))

$$\begin{aligned}\chi_\beta(\tau) &= \frac{1}{\beta}\chi_1(\tau/\beta), \quad \chi_1(\tau) = \frac{1}{\sqrt{2\pi}}\int \hat\chi(t)e^{i\tau t}\,dt,\\ g^{(\beta)}(\tau) &= \int g(\tau-\nu)\chi_\beta(\nu)\,d\nu = \int g(\nu)\chi_\beta(\tau-\nu)\,d\nu,\end{aligned}$$

where

$$\begin{aligned}&\hat\chi \in C_0^\infty(-T,T), \quad T \le T_0\\ &\hat\chi(-t) = \hat\chi(t) \in \mathbb{R} \text{ and } \hat\chi(t) = \frac{1}{\sqrt{2\pi}} \quad \text{for } |t| \le T/2.\end{aligned}$$

This, and the estimate (5.21) in Lemma 5.10 (valid for all $|t| \le T_0$) gives us (since $U_\beta(t;H) = e^{\frac{i}{\beta}Ht}$), that

$$\begin{aligned}\|\psi\, f(H)\,\chi_\beta(A-\lambda) &- \psi\, f(H)\,\chi_\beta(H-\lambda)\|_1\\ &= \left\| \frac{1}{\beta\sqrt{2\pi}}\int \hat\chi(t)\psi\, f(H)\,[U_\beta(t;A) - U_\beta(t;H)]\,dt \right\|_1\\ &\le \frac{C}{\beta\sqrt{2\pi}}\int_{-T_0}^{T_0} \left\|\psi\, f(H)\,[U_\beta(t;A) - U_\beta(t;H)]\right\|_1 dt\\ &\le \frac{2T_0}{\beta\sqrt{2\pi}}\,C_N\alpha^{-3/2}\beta^N = \tilde C_N\alpha^{-3/2}\beta^{N-1}.\end{aligned}$$

The estimate (5.28) now follows from the similar estimate (5.17) for the operator H (since $\alpha \in]0, \alpha_0]$).

Similarly,

$$\begin{aligned}
&\|\psi\, f(H)\, g^{(\beta)}(A) - \psi\, f(H)\, g^{(\beta)}(H)\|_1 \\
&\qquad \le \int \|g(\nu)\|\, \|\psi\, f(H)\, \chi_\beta(A-\nu) - \psi\, f(H)\, \chi_\beta(H-\nu)\|_1\, d\nu \\
&\qquad \le \tilde{C}_N \alpha^{-3/2}\beta^{N-1}\|g\|_{L^1}
\end{aligned}$$

by the computation above (since, by assumption, the 'non-critical' condition (5.27) holds for all $\lambda \in \operatorname{supp} g$). As before, the estimate (5.29) now follows from the result (5.18) for the operator H, and so this finishes the proof of the lemma. $\square$

We now move to the proof of Theorem 5.4. The idea is to derive it from the results in the previous lemma, by aid of the Tauberian argument in Proposition A.12.

Assume first that g is compactly supported, that is, $g \in C_0^{\infty,s}$. Also, assume that the condition (5.27) is satisfied for all $\lambda_0 \in \operatorname{supp} g$. Note, that with $\delta \le c/2$ (with c from (5.27)), the condition

$$|V(x) - \lambda| + |\partial V(x)|^2 \ge c/2 > 0, \qquad \forall x \in B(2E). \tag{5.31}$$

is fulfilled for all λ in the set

$$\mathcal{F}(\delta) = \{\lambda \mid \operatorname{dist}\{\operatorname{supp} g, \lambda\} \le \delta\}$$

since, for $\lambda \in D(\delta)$ and $\lambda_0 \in \operatorname{supp} g$ such that $\operatorname{dist}\{\operatorname{supp} g, \lambda\} = |\lambda - \lambda_0|$, we have

$$\begin{aligned}
|V(x) - \lambda| + |\partial V(x)|^2 &\ge |V(x) - \lambda_0| - |\lambda - \lambda_0| + |\partial V(x)|^2 \\
&\ge c - \delta \ge c/2 > 0.
\end{aligned}$$

Let now $\psi_1 \in C_0^\infty(\mathbb{R}^3)$ be a function such that $\psi\psi_1 = \psi$ (that is, $\psi_1 = 1$ on $\operatorname{supp}\psi$). Then, by Lemma B.16 (with $\chi = \psi_1^2$ and $g = f^2$)

$$\|\psi_1^2 f^2(A)\|_1 \le C\,\alpha^{-3/2}\beta^{-3} + C_N\alpha^{-2}\beta^N \quad \text{for all } N > 0,$$

such that, with $B^* = \psi_1\, f(A)$, we have

$$\|B^*B\|_1 \le C\,\alpha^{-3/2}\beta^{-3} + C_N\alpha^{-2}\beta^N \quad \text{for all } N > 0.$$

Also, by (2) in Lemma 5.11 and (3.1), we have the bound

$$\begin{aligned}
\|B^*\chi_\beta(A-\lambda)B\|_1 &= \|\psi_1\, f(A)\chi_\beta(A-\lambda)f(A)\psi_1\|_1 \\
&\le \|\psi_1\, f(A)\chi_\beta(A-\lambda)\|_1\|f(A)\psi_1\| \\
&\le C\,\beta^{-3} + C_N\alpha^{-2}\beta^N \quad \text{for all } N > 0
\end{aligned}$$

for all $\lambda \in \mathcal{F}(\delta)$ (since, by the spectral theorem, $\|f(A)\psi_1\| \le C$, independently of α and β). This means, that the condition for applying the Tauberian argument (Proposition A.12), the bound (A.21), is satisfied, with $Z(\beta) = \beta^{-3} + C_N\,\alpha^{-2}\beta^N$ for all $N \in \mathbb{N}$. Applying the Tauberian theorem, we get that

$$\begin{aligned}
&\|\psi_1\, f(A)[g(A) - g^{(\beta)}(A)]f(A)\,\psi_1\|_1 \\
&\qquad\qquad = \|\psi\psi_1\, f(A)[g(A) - g^{(\beta)}(A)]f(A)\,\psi_1\|_1 \\
&\qquad\qquad \le C\,\beta^{1+s}Z(\beta) + C_{N_1}\beta^{N_1}\|B^*B\|_1 \qquad \text{for all } N_1 > 0 \\
&\qquad\qquad \le C'\,\beta^{s-2} + C_N\alpha^{-2}\beta^N \qquad\qquad\quad\; \text{for all } N > 0.
\end{aligned}$$

Using the cyclicity of the trace, this means (since $\psi\psi_1^2 = \psi$) that

$$\|\psi f^2(A)[g(A) - g^{(\beta)}(A)]\|_1 \le C\,\beta^{s-2} + C_N\alpha^{-2}\beta^N \quad \text{for all } N > 0,$$

and so (since $fg = g$)

$$\begin{aligned}
\operatorname{Tr}\{\psi\, g(A)\} &= \operatorname{Tr}\{\psi\, f^2(A)g^{(\beta)}(A)\} \\
&\qquad\qquad + \mathcal{O}(\beta^{s-2}) + \mathcal{O}(\alpha^{-2}\beta^N) \quad \text{for all } N > 0.
\end{aligned}$$

The formula (5.5) now follows from the asymptotics of $\operatorname{Tr}\{\psi\, f^2 g^{(\beta)}\}$ in (5.29) (recall that $s \in [0,1]$ and $\beta \in]0, \beta_0]$).

Next, assume still that $g \in C_0^{\infty,s}$, but that the condition (5.4) holds:

$$|V(x)| + |\partial V(x)|^2 \ge c > 0, \qquad \forall x \in B(2E). \tag{5.32}$$

The idea is to split the function g in two, one that is C_0^∞ and so easy to treat (by (5.26) in Lemma 5.11) and one that has small support around zero, which can be treated by the above procedure; more explicitely, write

$$g = g_1 + g_2, \quad g_1 \in C_0^\infty(\mathbb{R}), \quad g_2 \in C_0^{\infty,s}(\mathbb{R}), \quad \operatorname{supp} g_2 \subset [-\varepsilon, \varepsilon].$$

As mentioned, the formula (5.5) for g_1 follows from (1) in Lemma 5.11, since $g_1 \in C_0^\infty(\mathbb{R})$. For $\varepsilon \le c/2$ (with c from the condition (5.32)) we have, for $\lambda \in \operatorname{supp} g_2 \subset [-\varepsilon, \varepsilon]$

$$|V(x) - \lambda| + |\partial V(x)|^2 \ge |V(x)| + |\partial V(x)|^2 - \lambda \ge c - \varepsilon \ge c/2 > 0$$

and so the condition (5.27) is fulfilled for all $\lambda \in \operatorname{supp} g_2$; the formula (5.5) for g_2 then follows from the argument above; adding up the results for g_1 and g_2 gives (5.5) for $g \in C_0^{\infty,s}$, with the condition (5.4) in the theorem.

To finally prove the theorem for general $g \in C^{\infty,s}$, we use the fact that the operator H is bounded from below by $-\|V\|_\infty$. To this end, split g again, this time in

$$g = g' + g'', \quad g' \in C^\infty(\mathbb{R}) \cap C^{\infty,1}(\mathbb{R}), \quad g'' \in C_0^{\infty,s}(\mathbb{R}).$$

The formula (5.5) for g'' was proved above, whereas, using the semi-boundedness of H, we can assume, that $g'(H) = 0$ (choose g' above such that $\operatorname{supp} g' \cap [-\|V\|_\infty, \infty[= \emptyset)$. Then, by the estimate (B.73) in Theorem B.18,

$$\begin{aligned}
&\operatorname{Tr}\{\psi\, g'(A)\} \\
&\qquad = \operatorname{Tr}\{\psi\, g'(H)\} + \mathcal{O}(\alpha^{-2}\beta^N) \quad \text{for all } N > 0 \\
&\qquad = \mathcal{O}(\alpha^{-2}\beta^N) \quad \text{for all } N > 0,
\end{aligned}$$

and so

$$\begin{aligned}
\operatorname{Tr}\{\psi\, g(A)\} &= \operatorname{Tr}\{\psi\, g'(A)\} + \operatorname{Tr}\{\psi\, g''(A)\} \\
&= \operatorname{Tr}\{\psi\, g''(A)\} + \mathcal{O}(\alpha^{-2}\beta^N) \quad \text{for all } N > 0 \\
&= \frac{1}{(2\pi\beta)^3} \int \psi(x) g''(a_\alpha(x,p))\, d^3x\, d^3p \\
&\qquad\qquad + \mathcal{O}(\beta^{s-2}) + \mathcal{O}(\alpha^{-2}\beta^N) \quad \text{for all } N > 0 \\
&= \frac{1}{(2\pi\beta)^3} \int \psi(x) g(a_\alpha(x,p))\, d^3x\, d^3p \\
&\qquad\qquad + \mathcal{O}(\beta^{s-2}) + \mathcal{O}(\alpha^{-2}\beta^N) \quad \text{for all } N > 0,
\end{aligned}$$

since $g'(a_\alpha(x,p)) = 0$ as

$$a_\alpha(x,p) \geq -\|V\|_\infty \quad \text{and} \quad \operatorname{supp} g' \subset]-\infty, -\|V\|_\infty].$$

This finishes the proof of theorem 5.4.

6. Multi-scale Analysis

In this section, we wish to apply the method of Multi-scale Analysis invented by Ivriĭ [17] (see also Ivriĭ [18] and Sobolev [38]) to the Herbst-operator. The idea of this procedure is to remove the non-critical condition (5.7) from Theorem 5.4 in the case of the specific functions g_s; also, the method alllows us (in this case) to get explicit control of the remainder. To this end, let

$$H(\beta, \alpha, V) = \sqrt{-\alpha^{-1}\beta^2\Delta + \alpha^{-2}} - \alpha^{-1} + V(x),$$

which is the quantisation of

$$a_\alpha(x,p) = \sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1} + V(x)$$

by $p \to -i\beta\nabla$.

The idea of Multi-scale Analysis is the following: when studying the local trace $\operatorname{Tr}\{\psi\, g(H)\}$ for $\psi \in C_0^\infty(D)$, one introduces two scales (apart from the semi-classical scale β): one will measure the size of the potential V in D, the other will measure the variation of V and ψ in D. Both of these scales will be functions on the set D and not merely constants. One then uses the variation-scale to construct a covering of D by open balls and a corresponding partition of unity, hereby reducing the problem to studying the local trace on these balls. It will be important, that the number of balls each ball overlaps with is bounded by a constant. The local trace on each ball is transformed into a scaled problem on a ball of a given size, by translation and dilation. The problem on this ball will be the 'model-problem': one assume that on this ball, one has an estimate on the difference between the local trace and the leading term in the asymptotics (the Weyl-term) as a function r, depending on α and β, but with a certain uniformity in ψ and V. As 'model-problem' will be used the result of Theorem 5.4 By the above procedure, one transforms this estimate into an estimate for the problem on D, which involves r as a function of the, by the two scales above, (continuously) scaled versions of the parameters α and β, integrated over the set D (by summing over the balls). For a good account on this procedure, see also Sigal [35].

To be more precise, for $D \subset \mathbb{R}^3$ an open set, assume given two strictly positive functions, $f \in C(\bar{D})$ and $l \in C^1(\bar{D})$, and assume that there exists numbers ϱ, c_1 and c_2, such that:

$$|\nabla l(x)| \leq \varrho < 1, \quad x \in D \tag{6.1}$$

$$c_1\, f(y) \leq f(x) \leq c_2\, f(y) \text{ for all } x \in D \cap B(y, l(y)), \quad y \in D. \tag{6.2}$$

That is, the function l does not vary too much (less than $|x|$) and locally, on a ball centrered at y, with radius $l(y)$, the variation of the function f is uniformly controlled by the two constants c_1 and c_2; that is, f does not vary too much on the scale of l.

Assume that '$A = H$ on D' in the sense, that A satisfies Assumption 5.1 with the open set D and assume, that the functions V and ψ satisfy

$$|\partial_x^m V(x)| \leq C_m\, f(x)^2\, l(x)^{-|m|}, \tag{6.3}$$

$$|\partial_x^m \psi(x)| \leq C_m\, l(x)^{-|m|} \tag{6.4}$$

for all $x \in D$ and $|m| \geq 0$. As mentioned above, one should think of the function f — or rather f^2 — as measuring the size of the potential V and the function l as measuring the way the potential V and the function ψ behave under differentiation (in the set D, that is).

Define for $s \in [0,1]$ the functions

$$g_s(\lambda) = \begin{cases} |\lambda|^s, & \lambda \leq 0 \\ 0, & \lambda > 0. \end{cases}$$

We will now study how the operators A and $H(\beta, \alpha)$, as well as the trace $\mathrm{Tr}\{\, \psi\, g_s(H(\beta, \alpha, V))\}$ and the Weyl-term, behave under translation and dilation. To this end, define, for $f, l > 0$, $z \in \mathbb{R}^3$:

$$\hat{V}(x) = f^{-2} V(lx + z)$$

and look at the dilation operator defined by

$$\big(\mathcal{U}_l u\big)(x) = l^{3/2} u(lx).$$

Then

$$\|\mathcal{U}_l u\|^2 = (\mathcal{U}_l u, \mathcal{U}_l u) = \int_{\mathbb{R}^3} |\mathcal{U}_l u(x)|^2 \, d^3x$$
$$= \int_{\mathbb{R}^3} |u(lx)|^2 l^3 \, d^3x = \int_{\mathbb{R}^3} |u(y)|^2 \, d^3y = \|u\|^2,$$

and so $\mathcal{U}_l$ is unitary and its adjoint is given by

$$\big(\mathcal{U}_l^* u\big)(x) = l^{-3/2} u(l^{-1}x).$$

Define also the translation operator by

$$\big(\mathcal{T}_z u\big)(x) = u(x+z).$$

Then obviously,

$$\big(\mathcal{T}_z^* u\big)(x) = u(x-z)$$

and also $\mathcal{T}_z$ is unitary.

We now wish to study the operator

$$f^{-2}\big(\mathcal{U}_l \mathcal{T}_z\big) A \big(\mathcal{U}_l \mathcal{T}_z\big)^*.$$

The aim is to show, that this operator equals a Herbst-operator, with rescaled β, α and V in a rescaled domain—the idea being, as mentioned in the introduction of the section, to transform any problem in a ball into a 'model problem' on a fixed ball by the above translation and dilation. Firstly, we claim that with

$$\hat{D} = \{x \in \mathbb{R}^3 \mid lx + z \in D\}$$

the operator $\big(\mathcal{U}_l \mathcal{T}_z\big)^*$ maps $C_0^\infty(\hat{D})$ into $C_0^\infty(D)$. To see this, let $\psi \in C_0^\infty(\hat{D})$. Then

$$\Big(\big(\mathcal{U}_l \mathcal{T}_z\big)^* \psi\Big)(x) = \Big(\mathcal{T}_z^* \mathcal{U}_l^* \psi\Big)(x) = \big(\mathcal{U}_l^* \psi\big)(x-z) = l^{-3/2}\psi(l^{-1}(x-z)).$$

Now, this is obviously C_0^∞, and if

$$\Big(\big(\mathcal{U}_l \mathcal{T}_z\big)^* \psi\Big)(x) \neq 0$$

then $l^{-1}(x-z) \in \hat{D}$, which means exactly that $x \in D$, so that $\operatorname{supp} \big(\mathcal{U}_l \mathcal{T}_z\big)^* \psi \subset D$.

This means, that $H(\beta, \alpha, V)$ and A agree on $\big(\mathcal{U}_l \mathcal{T}_z\big)^* \psi$ for $\psi \in C_0^\infty(\hat{D})$ (see (2) in Assumption 5.1) and so, with $\mathcal{M}(f)$ being multiplication by the function f and $\mathcal{F}$ being the Fourier transform, we have:

$$\begin{aligned}
&\Big((\mathcal{U}_l \mathcal{T}_z) A (\mathcal{U}_l \mathcal{T}_z)^* \psi \Big)(x) = l^{3/2} \Big(\mathcal{T}_z A (\mathcal{T}_z^* \mathcal{U}_l^*) \psi \Big)(lx) \\
&\quad = l^{3/2} \Big(A \mathcal{T}_z^* \mathcal{U}_l^* \psi \Big)(lx+z) = l^{3/2} \Big(H \mathcal{T}_z^* \mathcal{U}_l^* \psi \Big)(lx+z) \\
&\quad = l^{3/2} \Big(\mathcal{F}^{-1} \mathcal{M}(\sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1}) \mathcal{F} \mathcal{T}_z^* \mathcal{U}_l^* \psi \Big)(lx+z) \\
&\qquad + l^{3/2} \Big(\mathcal{M}(V) \mathcal{T}_z^* \mathcal{U}_l^* \psi \Big)(lx+z) \\
&\quad = l^{3/2} \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{i(lx+z)p} \Big(\mathcal{M}(\sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1}) \mathcal{F} \mathcal{T}_z^* \mathcal{U}_l^* \psi \Big)(p) \, d^3p \\
&\qquad + l^{3/2} V(lx+z) l^{-3/2} \psi(l^{-1}((lx+z)-z)) \\
&\quad = l^{3/2} \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{iz} e^{ix(lp)} \big(\sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1} \big) \big(\mathcal{F} \mathcal{T}_z^* \mathcal{U}_l^* \psi \big)(p) \, d^3p \\
&\qquad + V(lx+z) \psi(x).
\end{aligned}$$

Now, since

$$\begin{aligned}
\big(\mathcal{F} \mathcal{T}_z^* \mathcal{U}_l^* \psi \big)(p) &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{-ixp} \big(\mathcal{T}_z^* \mathcal{U}_l^* \psi \big)(x) \, d^3x \\
&= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{-ixp} l^{-3/2} \psi(l^{-1}(x-z)) \, d^3x \\
&= l^{3/2} e^{-iz} \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{-iy(lp)} \psi(y) \, d^3y \\
&= l^{3/2} e^{-iz} \big(\mathcal{F}\psi \big)(lp)
\end{aligned}$$

we get that

$$\begin{aligned}
&f^{-2} \Big((\mathcal{U}_l \mathcal{T}_z) A (\mathcal{U}_l \mathcal{T}_z)^* \psi \Big)(x) \\
&\quad = f^{-2} \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{ix(lp)} \big(\sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1} \big) \big(\mathcal{F}\psi \big)(lp) l^3 \, d^3p \\
&\qquad + f^{-2} V(lx+z) \psi(x) \\
&\quad = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{ixq} \big(\sqrt{-(\alpha f^2)^{-1} (\tfrac{1}{fl})^2 q^2 + (\alpha f^2)^{-2}} \\
&\qquad\qquad - (\alpha f^2)^{-1} \big) \big(\mathcal{F}\psi \big)(q) \, d^3q + \hat{V}(x) \psi(x) \\
&\quad = \Big(\big(\sqrt{-(\alpha f^2)^{-1} (\tfrac{\beta}{fl})^2 \Delta + (\alpha f^2)^{-2}} - (\alpha f^2)^{-1} + \hat{V}(x) \big) \psi \Big)(x) \\
&\quad \equiv \Big(H(\frac{\beta}{fl}, \alpha f^2, \hat{V}) \, \psi \Big)(x).
\end{aligned}$$

That is,

$$f^{-2} (\mathcal{U}_l \mathcal{T}_z) A (\mathcal{U}_l \mathcal{T}_z)^* = H(\tilde{\beta}, \tilde{\alpha}, \hat{V}) \quad \text{on} \quad C_0^\infty(\hat{D}),$$

with the rescaled parameters

$$\tilde{\beta} = \frac{\beta}{fl} \quad \text{and} \quad \tilde{\alpha} = \alpha f^2. \tag{6.5}$$

By the unitary equivalence of trace, we immediately get that

$$\mathrm{Tr}\{\,\psi\, g_s(H(\beta,\alpha,V))\} = f^{2s}\,\mathrm{Tr}\{\,\hat{\psi}\, g_s(H(\tilde{\beta},\tilde{\alpha},\hat{V}))\} \tag{6.6}$$

Note the similarity with Sobolev [38], (see also Sigal [35] for the non-magnetic case) where, given that an operator B agrees with the magnetic, non-relativistic Schrödinger operator (the function $a(x) = (a_1(x), a_2(x), a_3(x))$ being the magnetic vector potential):

$$T(h,\mu,V) = \sum_{l=1}^{3} \big(-ih\partial_{x_l} - \mu a_l\big)^2 + V$$

on $C_0^\infty(D)$, then

$$f^{-2}\big(\mathcal{U}_l\mathcal{T}_z\big)B\big(\mathcal{U}_l\mathcal{T}_z\big)^* = T\Big(\frac{h}{fl}, \frac{\mu l}{f}, \hat{V}\Big) \quad \text{on} \quad C_0^\infty(\hat{D}).$$

This is, as mentioned in section 4, the reason for our unusual choice of symbol, a_α, since it will allow us to use the Multi-scale Analysis for the non-relativistic case (invented by Ivriĭ [17]; see also Ivriĭ [18] and the references above) without major modifications; one difference is, that instead of the parameter μ, measuring the strength of the magnetic field, we have α, measuring the 'degree of relativity', so to speak.

About the leading term $\mathfrak{W}_s(\beta,\alpha,\psi,V)$ in the asymptotics of $\mathrm{Tr}\{\,\psi\, g_s(H(\beta,\alpha,V))\}$ we only need few facts. Firstly, it need to scale like $\mathrm{Tr}\{\,\psi\, g_s(H(\beta,\alpha,V))\}$, secondly, it should be additive in the function ψ. That the Weyl-term

$$\begin{aligned}
&\mathfrak{W}_s(\beta,\alpha,\psi,V) \\
&\qquad = (2\pi\beta)^{-3} \iint \psi(x)\,\big|\sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1} + V(x)\big|_-^s \, d^3x\, d^3p
\end{aligned}$$

is linear in ψ is obvious, and

$$\begin{aligned}
&\mathfrak{W}_s(\tilde{\beta},\tilde{\alpha},\hat{\psi},\hat{V}) \\
&\quad = \frac{(fl)^3}{(2\pi\beta)^3} \iint \psi(lx+z)\big|\sqrt{(\alpha f^2)^{-1}p^2 + (\alpha f^2)^{-2}} \\
&\qquad\qquad\qquad\qquad - (\alpha f^2)^{-1} + f^{-2}V(lx+z)\big|_-^s \, d^3x\, d^3p \\
&\quad = f^{-2s}(2\pi\beta)^{-3} \iint \psi(y)\big|\sqrt{\alpha^{-1}q^2 + \alpha^{-2}} - \alpha^{-1} + V(y)\big|_-^s \, d^3y\, d^3q \\
&\quad = f^{-2s}\mathfrak{W}_s(\beta,\alpha,\psi,V)
\end{aligned} \tag{6.7}$$

by the changes of variables, $y = lx + z$ and $q = fp$.

We now move on to the assumptions on the 'model-problem':

Firstly, we need to generalise the 'non-critical condition' (5.7). Let $F = F(t,x)$, $t \in \mathbb{R}$, $x \in \mathbb{R}^3$, be a real-valued function such that

$$F(\tau t, \tau^{\frac{1}{2}} x) = \tau F(t,x), \text{ for all } \tau > 0. \tag{6.8}$$

The 'generalised non-critical condition' is then the assumption, that

$$F(\,|W(x)| + \beta, \partial_x W(x)) \geq \kappa, \text{ for all } x \in B(4) \tag{6.9}$$

for some $\kappa \geq 0$. Note that by the definitions of $\tilde{\beta}$, $\hat{\psi}$ and $\hat{V}$ and the scaling (6.8) we get that

$$\begin{aligned} F(\,|\hat{V}(x)| + \tilde{\beta}, \partial_x \hat{V}(x)) &= F(f^{-2}|V(y)| + \frac{\beta}{fl}, lf^{-2}\partial_y V(y))\Big|_{y=lx+z} \\ &= f^{-2} F(\,|V(y)| + \frac{\beta f}{l}, \frac{l}{f}\partial_y V(y))\Big|_{y=lx+z}. \end{aligned} \tag{6.10}$$

Assumption 6.1. *Assume, that the operator A satisfies Assumption 5.1 with $D = B(8)$, a potential W, and $\beta \in]0,\beta_0]$, $\alpha \in]0,\alpha_0]$ for some fixed β_0 and α_0. Assume further, that the 'generalised non-critical condition' (6.9) is satisfied. Then there exists a locally bounded, positive function $r(\beta,\alpha)$, uniform in W and ϕ satisfying*

$$|\partial^m W(x)| \leq C_m \quad , \quad |\partial^m \phi(x)| \leq C_m \quad , \quad \forall m \in \mathbb{N}^3 \quad , \quad \forall x \in B(8), \tag{6.11}$$

such that

$$\Big|\operatorname{Tr}\{\,\phi\, g_s(A)\} - \mathfrak{W}_s(\beta,\alpha,\phi,W)\Big| \leq r(\beta,\alpha). \tag{6.12}$$

Remark 6.2. The idea is that given one estimate — a 'modelproblem' — as the one in the assumption above, we will, by the Multi-scale Analysis, prove one without the (generalised) non-critical condition on the symbol: it will simply be 'scaled away' (see Sigal [35] for more on the 'philosophy' of the method). Note, that due to Theorem 5.4, Assumption 6.1 is valid with $F(t,x) = t + |x|^2$ and $r(\beta,\alpha) = C\,\beta^{s-2} + C_N \alpha^{-2}\beta^N$.

To apply this to the general operator A, we need to impose further restrictions on the scale-functions f and l, and on the potential V: assume that

$$\beta_0\, f(x)\, l(x) \geq \beta \quad , \quad \alpha f(x)^2 \leq \alpha_0, \quad x \in D, \tag{6.13}$$

and that, for some $\omega > 0$ (and the same κ as in Assumption 6.1)

$$F\Big(\,|V(x)| + \frac{\beta f(x)}{l(x)}, \frac{l(x)}{f(x)}\partial_x V(x)\Big) \geq \omega\kappa f(x)^2, \quad x \in D. \tag{6.14}$$

The relevance of this assumption should be clear from (6.10). Lastly, we need to assume, that if the ball at $x \in D$ with radius $l(x)$ touches supp ψ, then the ball that is eight times as big stays within D:

$$\bigcup_{x\in\Omega} B(x, 8\,l(x)) \subset D$$

with

$$\Omega = \{x \in D \mid B(x, l(x)) \cap \operatorname{supp}\psi \neq \emptyset\}.$$

One could say that this means that the support of ψ is much smaller than D, on scales measured by the function l.

As mentioned earlier, the idea is to split the general problem (with varying scales f and l) into problems on a number of balls (with fixed, but different scales) by constructing a covering of D — and a partition of unity, subordinate this covering — using the scale-function l. This done, the above ensures that for the balls we need to take into account (namely, the ones that touches the support of the function ψ), the scaled ball, with a radius eight times as big, will still stay within D.

Firstly, we now look at what happens on an arbitrary ball.

Lemma 6.3. *Let the operator A satisfy Assumption 5.1 with $D = B(z, 8\,l)$ for some $z \in \mathbb{R}^3$ and $l > 0$. Assume furthermore, that the scaling conditions (6.3), (6.4) and (6.13) are fulfilled with $\psi \in C_0^\infty(B(z,l))$ and the scaling functions equalling constants:*

$$f(x) = f > 0 \quad \text{and} \quad l(x) = l > 0.$$

Finally, assume that the 'generalised non-critical condition' (6.14) is satisfied for the potential V, with $\omega = 1$:

$$F\Big(\,|V(x)| + \frac{\beta f}{l}, \frac{l}{f}\partial_x V(x)\Big) \geq \kappa f^2, \quad x \in D. \tag{6.15}$$

Assume that Assumption 6.1 holds. Then

$$\Big|\operatorname{Tr}\{\,\phi\, g_s(A)\} - \mathfrak{W}_s(\beta, \alpha, \phi, W)\Big| \leq f^{2s}\, r\Big(\frac{\beta}{fl}, \alpha f^2\Big). \tag{6.16}$$

Proof. This is a simple consequence of the way we have set up things; it all comes down to scaling. Note that due to (6.13) we have that

$$\tilde\beta = \frac{\beta}{fl} \leq \beta_0, \quad \tilde\alpha = \alpha f^2 \leq \alpha_0.$$

Also, by the definition of the potential $\hat V$ and the assumption (6.3) on the potential V in $B(z, 8\,l)$, we have that

$$|\,\partial_x^m \hat V(x)| = |\,l^{|m|}(\partial_x^m V)(lx+z)| \leq l^{|m|} C_m l^{-|m|} = C_m,$$

for $lx + z \in B(z, 8\,l)$, that is, $W = \hat V$ satisfies (6.11) in the ball $B(0,8)$; likewise, by the assumption (6.4) on ψ, $\phi = \hat\psi$ satisfies (6.11) in the same ball. Lastly, by the calculation (6.10) and the assumption (6.15) we get that

$$F\Big(\,|\hat V(x)| + \tilde\beta, \partial_x \hat V(x)\Big) \geq \kappa, \quad x \in B(0,8).$$

This way, all the prerequisites for using Assumption 6.1 are satisfied, and

$$\Big|\,\mathrm{Tr}\{\,\hat\phi\, g_s(A(\tilde\beta,\tilde\alpha,\hat V))\} - \mathfrak{W}_s(\tilde\beta,\tilde\alpha,\hat\phi,\hat V)\Big| \le r(\tilde\beta,\tilde\alpha).$$

Now the lemma follows by the scaling properties (6.6) and (6.7) of the trace-term, resp. the leading-order term, and by the definition of $\tilde\beta$ and $\tilde\alpha$ (see (6.5)). □

To treat the general problem, we need to construct a covering of D and a partition of unity, subordinate to that covering. This is done using the scale function l in exactly the same way as in Sobolev [38]: we observe that due to the slow variation of l, see (6.1), we can regard $l = l(x)$ as a function that defines a *slowly varying metric* in D (see Hömander [15, Def. 1.4.7]), which first gives us a covering of the set D and then a very specific partition of unity, subordinate this covering; see Sobolev [38, Lemma 5.4].

Lemma 6.4. *Let the function $l \in C^1(\bar D)$ satisfy*

$$|\nabla l(x)| \le \varrho, \quad x \in D$$

for some $\varrho < 1$. Then

(1) There exists a sequence $\{x_k\}_{k\in\mathbb{N}} \subset D$ such that the open balls $B(x_k, l(x_k))$ form a covering of D, that is,

$$D \subset \bigcup_k B(x_k, l(x_k)).$$

There exists a number, $N = N_\varrho$, depending only on the constant ϱ above, such that the intersection of more than N_ϱ balls is empty.

(2) One can choose a sequence $\{\psi_k\}_{k\in\mathbb{N}}$ of functions,

$$\psi_k \in C_0^\infty(B(x_k, l(x_k))), \quad k = 1, 2, \dots$$

such that

$$|\,\partial_x^m \psi_k(x)| \le C_m\, l(x_k)^{-|m|}, \text{ for all } k = 1, 2, \dots \quad , \tag{6.17}$$

and

$$\sum_k \psi_k(x) = 1, \quad x \in D. \tag{6.18}$$

The constants C_m in (6.17) depend only on the constant ϱ.

As mentioned earlier, the idea is to use the partition to cut down the potential V and the cut-off function ψ to potentials and functions on each ball $B_k = B(x_k, l(x_k))$, by aid of (6.17) each satisfying estimates like (6.3) and (6.4) with $l(x) = l(x_k)$ and $f(x) = l(f_k)$ (with new constants, which only depend on the old ones and the partition), so that we can apply Lemma 6.3.

Firstly, let

$$\mathfrak{B} = \{k \in \mathbb{N} \,|\, \operatorname{supp} \psi \cap B_k \neq \emptyset\,\}. \tag{6.19}$$

Then, by linearity and (6.18)

$$\operatorname{Tr}\{\psi\, g_s(A)\} = \sum_{k\in\mathfrak{B}} \operatorname{Tr}\{\psi\psi_k\, g_s(A)\} \tag{6.20}$$

and

$$\mathfrak{W}_s(\beta,\alpha,\phi,V) = \sum_{k\in\mathfrak{B}} \mathfrak{W}_s(\beta,\alpha,\phi\psi_k,V) \tag{6.21}$$

The idea is to prove a bound on the difference (the 'error')

$$\operatorname{Tr}\{\psi\psi_k\, g_s(A)\} - \mathfrak{W}_s(\beta,\alpha,\phi\psi_k,V)$$

and then sum these for $k\in\mathfrak{B}$. We need a couple of definitions before stating our main result.

For the function r of Assumption 6.1 and any set $K\subset\bar{D}$, denote

$$\mathcal{R}(\beta,\alpha,K) = \int_K f(x)^{2s} r\left(\frac{\beta}{l(x)f(x)},\alpha f(x)^2\right) l(x)^{-3}\, d^3x. \tag{6.22}$$

Since $l\in C^1(\bar{D})$ is positive, this integral makes sense. Note that the arguments of the function r are the (continuously) re-scaled versions of β and α (see also (6.5)). To go from sums to integrals, we need the notion of a function of 'moderare variation':

Definition 6.5. A measurable function $f:\mathbb{R}^n\to\mathbb{C}$, $n\geq 1$, is said to be of *moderate variation* if, for almost all $x,y\in\mathbb{R}^n$:

$$\frac{1}{c_1}\leq\frac{|x|}{|y|}\leq c_1 \Rightarrow \frac{1}{c_2}\leq\frac{|f(x)|}{f|y|}\leq c_2$$

with a constant $c_2=c_2(c_1)$ depending on c_1.

This leads us to the main (abstract) result of this section.

Theorem 6.6. *Given an open set $D\subset\mathbb{R}^3$. Let the positive functions $l\in C^1(\bar{D})$ and $f\in C(\bar{D})$ satisfy*

$$|\nabla l(x)|\leq\varrho<1,\quad x\in D \tag{6.23}$$

$$c_1\, f(y)\leq f(x)\leq c_2\, f(y) \text{ for all } x\in D\cap B(y,l(y)),\quad y\in D \tag{6.24}$$

and let Assumption 6.1 be fulfilled for any functions W and ϕ satisfying

$$|\partial^m W(x)|\leq C_m \tag{6.25}$$

$$|\partial^m\phi(x)|\leq C_m\quad,\quad |m|\geq 0,\ x\in B(8), \tag{6.26}$$

with functions r and F of moderate variation on $B(8)$.

Let the operator A satisfy Assumption 5.1 for the open set D with a potential V satisfying

$$|\partial^m V(x)|\leq C_m f(x)^2 l(x)^{-|m|}\quad,\quad x\in D\quad,\quad |m|\geq 0 \tag{6.27}$$

and let $\psi\in C_0^\infty(D)$ satisfy

$$|\partial^m\psi(x)|\leq C_m l(x)^{-|m|}\quad,\quad x\in D\quad,\quad |m|\geq 0. \tag{6.28}$$

Assume furtermore, that

$$\beta_0 f(x) l(x) \geq \beta \quad \text{and} \quad \alpha_0 \geq f(x)^2 \alpha \quad , \quad x \in D \tag{6.29}$$

and that

$$F\Big(|V(x)| + \frac{\beta f(x)}{l(x)}, \frac{l(x)}{f(x)}\, \partial_x V(x)\Big) \geq \omega\kappa f(x)^2 \ , \ x \in D \tag{6.30}$$

for some $\omega > 0$ *sufficiently large and the* κ *from Assumption 6.1 (namely, such that* $F\big(|V(x)| + \beta, \partial_x V(x)\big) \geq \kappa \ , \ x \in D$*). Finally, assume that, with*

$$\mathfrak{G} = \{x \in D \mid B(x, l(x)) \cap \operatorname{supp} \psi \neq \emptyset\ \} \tag{6.31}$$

we have

$$\bigcup_{x \in \mathfrak{G}} B(x, 8l(x)) \ \subset D. \tag{6.32}$$

Then, with $\mathcal{R}$ *as in (6.22):*

$$\Big|\operatorname{Tr}\{\psi\, g_s(A) - \mathfrak{W}_s(\beta, \alpha, \phi, V)\Big| \leq C\, \mathcal{R}(\beta, \alpha, D). \tag{6.33}$$

The constant C *depends only on the constants* C_m *in (6.27) and (6.28), on* ϱ, c_1 *and* c_2 *in (6.24), and on* α_0, β_0 *and* ω.

Proof. As mentioned earlier, the idea is to use the partition $\{\psi_k\}_{k\in\mathbb{N}}$ from Lemma 6.4 and the expansions (6.20) and (6.21). For the sequence $\{x_k\}_{k\in\mathbb{N}} \subset D$ from Lemma 6.4 (constructed by aid of the function l from the theorem) let $l_k = l(x_k)$ and $f_k = f(x_k)$ for $k \in \mathfrak{B}$ (see (6.19)). This means by (6.32) that $B(x_k, 8l_k) \subset D$ and so that, by (6.24) and the definition of f_k:

$$x \in B(x_k, l_k) \quad \Rightarrow \quad c_1 f_k \leq f(x) \leq c_2 f_k \tag{6.34}$$

with constants independent of k. Furthermore, since

$$|\nabla l(x)| \leq \varrho < \frac{1}{8} \quad , \quad x \in D$$

and $B(x_k, 8l_k) \subset D$, we have that

$$\big|l_k - l(x)\big| \leq \varrho |x_k - x| \leq \varrho \cdot 8 l_k \quad \text{for all} \quad x \in B(x_k, 8l_k)$$

and so

$$\big(1 - 8\varrho\big) l_k \leq l(x) \leq \big(1 + 8\varrho\big) l_k. \tag{6.35}$$

Next, by Leibniz' rule, the property (6.17), and the assumption (6.28) on $\partial^m \psi$, we have that

$$\begin{aligned}\big|\partial^m\left(\psi\psi_k\right)\big| &\leq \sum_{|a|+|b|=|m|} c(a,b)\big|\partial^a\psi\, \partial^b\psi_k\big| \\ &\leq \sum_{|a|+|b|=|m|} c(a,b) C_a l(x)^{-|a|}\, l_k^{-|b|} \leq \tilde{C}\ l_k^{-|m|}.\end{aligned}$$

The last inequality by (6.35); the constant $\tilde{C}$ depends on ϱ, the constants in (6.28) and the ones in (6.17). Similarly, using (6.34), we get that (note the importance of $\varrho < 8$)

$$|\partial^m V(x)| \leq C_m f(x)^2 l(x)^{-|m|} \leq \left(C_m c_2^2 (1-8\varrho)^{-|m|}\right) f_k^2\, l_k^{-|m|}.$$

Since, by (6.34) and (6.35)

$$c_1 \leq \left|\frac{f(x)}{f_k}\right| \leq c_2 \quad \text{and} \quad \left(1-8\varrho\right) \leq \left|\frac{l(x)}{l_k}\right| \leq \left(1+8\varrho\right) \tag{6.36}$$

we have, as the function F by assumption is of moderate variation:

$$\tilde{c}_3 \leq \left|\frac{F(s,X)}{F(t,Y)}\right| \leq \tilde{C}_3$$

with

$$\begin{aligned} s &= |V(x)| + \frac{\beta f_k}{l_k} \quad , \quad X = \frac{l_k}{f_k}\, \partial_x V(x) \\ t &= |V(x)| + \frac{\beta f(x)}{l(x)} \quad , \quad Y = \frac{l(x)}{f(x)}\, \partial_x V(x) \end{aligned}$$

and so

$$\begin{aligned} F\Big(|V(x)| + \frac{\beta f_k}{l_k}, \frac{l_k}{f_k}\, \partial_x V(x)\Big) &\geq \tilde{c}_5 F\Big(|V(x)| + \frac{\beta f(x)}{l(x)}, \frac{l(x)}{f(x)} \partial_x V(x)\Big) \\ &\geq \tilde{c}_5 \big(\omega\kappa f(x)^2\big) \geq \tilde{c}_5 c_1^2\, \omega\kappa f_k^2 \qquad \text{for all } x \in B(x_k, 8l_k). \end{aligned}$$

Now all the conditions in Lemma 6.3 are satisfied for $l = l_k$ and $f = f_k$ (for sufficiently big ω) and therefore

$$\begin{aligned} \Big|\mathrm{Tr}\{\psi\psi_k\, g_s(A)\} - \mathfrak{W}_s(\beta,\alpha,\phi\psi_k,V)\Big| &\leq f_k^{2s} r\left(\frac{\beta}{l_k f_k}, \alpha f_k^2\right) \\ &= \int_{B_k} f_k^{2s} r\left(\frac{\beta}{l_k f_k}, \alpha f_k^2\right) \left(\frac{4\pi}{3}(8l_k)^3\right)^{-1} d^3x \\ &\leq C \int_{B_k} f(x)^{2s} r\left(\frac{\beta}{l(x) f(x)}, \alpha f(x)^2\right) l(x)^{-3}\, d^3x. \end{aligned}$$

The last inequality using that the function r is also assumed to be of moderate variation, and (6.36). This means that

$$\begin{aligned} &\Big|\mathrm{Tr}\{\psi\, g_s(A)\} - \mathfrak{W}_s(\beta,\alpha,\phi,V)\Big| \\ &\qquad \leq \sum_{k\in\mathfrak{B}} \Big|\mathrm{Tr}\{\psi\psi_k\, g_s(A) - \mathfrak{W}_s(\beta,\alpha,\phi\psi_k,V)\Big| \\ &\qquad \leq \sum_{k\in\mathfrak{B}} \hat{C}\, \mathcal{R}(\beta,\alpha,B_k) \leq \tilde{C}_\varrho\, \mathcal{R}(\beta,\alpha,D) \end{aligned}$$

(with a constant C_ϱ that depends on ϱ) since, by construction, there is an upper bound, N_ϱ, on the number of overlapping balls, see (1) in Lemma 6.4. This proves the theorem. $\square$

We are now ready to remove the non-critical condition (5.7) of Theorem 5.4 in the case of g_1:

Theorem 6.7. *Let* $\psi \in C_0^\infty(B(E/2))$ *satisfy*

$$|\partial^m \psi(x)| \le C_m \quad \forall m, \tag{6.37}$$

and let

$$g_1(\lambda) = \begin{cases} |\lambda|, & \lambda \le 0 \\ 0, & \lambda > 0. \end{cases}$$

Suppose that the operator A *satiesfies Assumption 5.1 with* $D = B(4E)$, $\alpha \in]0, \alpha_0]$, $\beta \in]0, \beta_0]$ *and a potential* $V \in C_0^\infty(\mathbb{R}^3)$ *that satisfies*

$$|\partial^m V(x)| \le C_m \quad \forall m. \tag{6.38}$$

Then

$$\begin{aligned} \operatorname{Tr}\{\psi\, g_1(A)\} = {} & \frac{1}{(2\pi\beta)^3} \int \psi(x)\, g_1(a_\alpha(x,p))\, d^3x\, d^3p \\ & + \mathcal{O}(\beta^{-1}) + \mathcal{O}(\alpha^{-2}\beta^N) \quad , \quad \textit{for all } N \in \mathbb{N}. \end{aligned} \tag{6.39}$$

Proof. We note that taking $E = 2$, Theorem 5.4 assures the validity of Assumption 6.1 with

$$\begin{aligned} F(t,x) &= t + |x|^2, \\ r_1(\beta,\alpha) &= C\,\beta^{-1} + C_N \alpha^{-2}\beta^N \quad \forall N. \end{aligned}$$

The functions F and r are clearly of moderate variation (see Definition 6.5), and F satisfies (6.8).

Next we note that Proposition D.17 assures the validity of Assumption 6.1 with same F as above (in fact, with $F \equiv 0$) and

$$r_2(\beta,\alpha) = C\,\beta^{-3}.$$

The idea is that we can take the minimum of r_1 and r_2 as our choice of r.

Define now

$$l(x) = A^{-1}\Big[V(x)^2 + \big(\partial_x V(x)\big)^4 + \beta^2\Big]^{1/4} \quad , \quad A > 0.$$

and $f(x) = b \cdot l(x)$, $b > 0$. Since $V \in C_0^\infty(\mathbb{R}^3)$ we have that $f, l \in C^\infty(\mathbb{R}^3)$ and f, l are positive (since $\beta > 0$). Also, for A big enough (depending on the constants C_m in (6.38)), l and f satisfy (6.23) and (6.24). Also for A big enough, we have (6.32), since $\operatorname{supp}\psi \subset B(E/2)$. Due to the conditions (6.37) and (6.38) and the definition of l and f, the estimates (6.27) and (6.28) are trivially satisfied. With $C_0 = \|V\|_\infty$ and $C_1 = \max_{|m|=1} C_m$ (see (6.26)), (6.29) is satisfied for $b < 2^{-1/4}$,

$\beta_0 \geq A^2 b$, $\beta_0^2 \geq C_0^2 + C_1^4$. Finally, as $f = b \cdot l$, the condition (6.30) reads:

$$\begin{aligned} F\Big(|V(x)| + \frac{\beta f(x)}{l(x)}, \frac{l(x)}{f(x)}\partial_x V(x)\Big) &= |V(x)| + b\,\beta + \frac{1}{b^2}|\partial_x V(X)|^2 \\ &\geq \omega\kappa f(x)^2 = \frac{\omega\kappa b^2}{A^2}\Big[|V(x)|^2 + \big(\partial_x V(x)\big)^4 + \beta^2\Big]^{1/2} \qquad (6.40) \end{aligned}$$

which is fulfilled choosing $\omega \leq A^2\kappa^{-1}b^{-1}$, due to the triangle inequality in $\mathbb{R}^3$ (since $b < 1$).

In this way, the conditions of Theorem 6.6 are all satisfied. We split the set D in two: where $f(x) \geq \beta^{2/5}$ — here we use the function r_1 — and where $f(x) \leq \beta^{2/5}$ — here we use r_2. More precisely, let

$$\begin{aligned} D_1 &= \big\{x \in D \,\big|\, f(x) \geq \beta^{2/5}\big\}, \\ D_2 &= \big\{x \in D \,\big|\, f(x) \leq \beta^{2/5}\big\}. \end{aligned}$$

Then, with $r = \min\{r_1, r_2\}$:

$$\mathcal{R}(\beta, \alpha, D) = C \int_D f(x)^2 r\Big(\frac{\beta}{f(x)l(x)}, \alpha f(x)^2\Big) l(x)^{-3}\, d^3x,$$

and so, since $f(x) \geq \beta^{2/5}$ on D_1 and $l(x) \geq \beta^{1/2}$ by construction,

$$\begin{aligned} \mathcal{R}(\beta, \alpha, D_1) &= C \int_{D_1} f(x)^2 r\Big(\frac{\beta}{f(x)l(x)}, \alpha f(x)^2\Big) l(x)^{-3}\, d^3x \\ &\leq C \int_{D_1} l(x)^2 r_1\Big(\frac{\beta}{f(x)l(x)}, \alpha f(x)^2\Big) l(x)^{-3}\, d^3x \\ &\leq C\,\beta^{-1}\int_D l(x)\, d^3x + C_N\alpha^{-2}\beta^N \int_D f(x)^{-2-N} l(x)^{-N-3}\, d^3x \\ &\leq C'\beta^{-1} + C'_N\alpha^{-2}\beta^{\frac{N}{10}-\frac{19}{10}}, \end{aligned}$$

since l is bounded. Given $\tilde{N}$, choosing $N = 10\tilde{N} + 20$, we have that

$$\mathcal{R}(\beta, \alpha, D_1) \leq C'\beta^{-1} + C'_N\alpha^{-2}\beta^{\tilde{N}}.$$

Secondly, remembering that $f = b \cdot l$ and that $f(x) \leq \beta^{2/5}$ on D_2:

$$\begin{aligned} \mathcal{R}(\beta, \alpha, D_2) &= C \int_{D_2} l(x)^2 r\Big(\frac{\beta}{f(x)l(x)}, \alpha f(x)^2\Big) l(x)^{-3}\, d^3x \\ &\leq C \int_{D_2} l(x)^2 r_2\Big(\frac{\beta}{f(x)l(x)}, \alpha f(x)^2\Big) l(x)^{-3}\, d^3x \\ &\leq C\,\beta^{-3}\int_{D_2} f(x)^5\, d^3x \leq C\,\beta^{-3+5\cdot\frac{2}{5}} = C\,\beta^{-1}. \end{aligned}$$

Since

$$\mathcal{R}(\beta, \alpha, D) = \mathcal{R}(\beta, \alpha, D_1) + \mathcal{R}(\beta, \alpha, D_2),$$

this proves the theorem. $\square$

Having shown this, we are ready for the result for a more general domain D. This follows by a 'bootstrapping' argument:

Theorem 6.8. *Given an open set $D \subset \mathbb{R}^3$. Let the positive functions $l \in C^1(\bar{D})$ and $f \in C(\bar{D})$ satisfy*

$$|\nabla l(x)| \leq \varrho < 1, \quad x \in D \tag{6.41}$$

$$c_1\, f(y) \leq f(x) \leq c_2\, f(y) \text{ for all } x \in D \cap B(y, l(y)), \quad y \in D. \tag{6.42}$$

Let the operator A satisfy Assumption 5.1 for the open set D, with $\alpha \in]0, \alpha_0]$ and $\beta \in]0, \beta_0]$, and with a potential V satisfying

$$|\partial^m V(x)| \leq C_m f(x)^2 l(x)^{-|m|} \quad , \quad x \in D \quad , \quad |m| \geq 0 \tag{6.43}$$

and let $\psi \in C_0^\infty(D)$ satisfy

$$|\partial^m \psi(x)| \leq C_m l(x)^{-|m|} \quad , \quad x \in D \quad , \quad |m| \geq 0. \tag{6.44}$$

Assume furtermore, that

$$\beta_0 f(x) l(x) \geq \beta \quad \text{ and } \quad \alpha_0 \geq f(x)^2 \alpha \quad , \quad x \in D$$

Finally, assume that, with

$$\mathfrak{G} = \{ x \in D \mid B(x, l(x)) \cap \operatorname{supp} \psi \neq \emptyset \}$$

we have

$$\bigcup_{x \in \mathfrak{G}} B(x, 8l(x)) \subset D. \tag{6.45}$$

Then

$$\begin{aligned} &\Big| \operatorname{Tr}\{\psi\, g_1(A) - \mathfrak{W}_1(\beta, \alpha, \phi, V) \Big| \\ &\qquad \leq C\, \beta^{-1} \int_D f(x)^3 l(x)^{-2}\, d^3x \\ &\qquad\qquad + C_N \alpha^{-2} \beta^N \int_D f(x)^{-2-N} l(x)^{-N-3}\, d^3x. \end{aligned} \tag{6.46}$$

The constant C depends on the constants C_m in (6.43) and (6.44), on ϱ, c_1 and c_2 in (6.42), and on α_0, β_0 and ω.

Proof. According to Theorem 6.7, the operator A satisfies Assumption 6.1, for $\alpha \in]0, \alpha_0]$ and $\beta \in]0, \beta_0]$, with

$$\begin{aligned} &F(t, x) \equiv 0, \\ &r(\beta, \alpha) = C\, \beta^{-1} + C_N \alpha^{-2} \beta^N \quad \text{ for all } N \geq 0. \end{aligned}$$

The result now follows from Theorem 6.6 and (6.22). □

We now employ the result from Theorem 6.8 for a spherical shell — more precisely:

Theorem 6.9. *Let* $\kappa \in [0,1]$. *Let* V *satisfy*

$$\left|\partial^m V(x)\right| \le C_m |x|^{-1-|m|} \quad , \quad \forall m, \tag{6.47}$$

and let $\psi \in C_0^\infty(\mathbb{R}^3)$ *with*

$$\operatorname{supp}\psi \subset \left\{\, x \mid r \le |x| \le \rho \right\} \quad , \quad 64^2 \le r \le \rho \le C\,\kappa^{-1},$$

and

$$\left|\partial^m \psi(x)\right| \le C_m |x|^{-|m|} \quad , \quad \forall |m| \ge 0 \quad , \quad \forall x \ne 0. \tag{6.48}$$

Then

$$\Bigg| \operatorname{Tr}\Big\{\, \psi \,\Big|\sqrt{p^2+1} - 1 - \frac{\delta}{|x|} - \kappa\Big|_- \Big\} - \frac{1}{(2\pi)^3} \iint d^3\!p\, d^3\!x \Big[\frac{p^2}{2} - \frac{\delta}{|x|} + \kappa\Big]_- \Bigg| \le C\, r^{-1/2}. \tag{6.49}$$

This is uniformly in V *and* ψ *in the sense that it only depends on the constants in (6.47) and (6.48).*

Proof. The idea is to use Theorem 6.8 with $\alpha = \alpha_0 = \beta = \beta_0 \equiv 1$ and $s = 1$. Let

$$f(x) = |x|^{-1/2} \quad , \quad l(x) = \varrho |x| \quad , \quad \frac{1}{32} < \varrho < \frac{1}{16}$$

and

$$D = \left\{\, x \in \mathbb{R}^3 \;\Big|\; \frac{r}{4} < |x| < 2\rho \right\}.$$

Then (6.23) is clearly satisfied and if $x \in D \cap B(y, l(y))$ for $y \in D$, then

$$\frac{r}{4} < |y| < 2\rho \quad \text{and} \quad |x-y| < l(y) < \frac{|y|}{16}$$

so

$$\frac{4}{\sqrt{17}}\, |y|^{-1/2} \le |x|^{-1/2} \le \frac{4}{\sqrt{15}}\, |y|^{-1/2}$$

and therefore f satiesfies (6.42) with

$$c_1 = \frac{4}{\sqrt{17}} \quad , \quad c_2 \frac{4}{\sqrt{15}}.$$

Also, if

$$B(x, l(x)) \cap \operatorname{supp}\psi \ne \emptyset$$

then either

$$|x| - l(x) \le \rho \quad \text{or} \quad |x| + l(x) \ge r.$$

This means that

$$\frac{16}{17}\, r < |x| < \frac{16}{15}\, \rho.$$

Now,

$$
\begin{aligned}
&y \in B(x, 8l(x)) \quad \Rightarrow \quad |x-y| < 8l(x) < \frac{1}{2}|x| \quad \Rightarrow \\
&\frac{r}{4} < \frac{8}{17}r < \frac{1}{2}|x| < |y| < \frac{3}{2}|x| < \frac{48}{30}\rho < 2\rho \quad \Rightarrow \quad y \in D
\end{aligned}
$$

and so

$$\bigcup_{x\in\mathfrak{B}} B(x, 8l(x)) \subset D$$

with

$$\mathfrak{B} = \big\{\, x \bigm| B(x, l(x)) \cap \operatorname{supp}\psi \neq \emptyset \big\}.$$

With the choice of the functions f and l, and since $r \geq 64^2$, we have:

$$\frac{\beta}{l(x)f(x)} = \frac{1}{\varrho|x|^{1/2}} < \frac{32}{\sqrt{r}} \leq 1 = \beta_0 \qquad \forall x \in D$$

and:

$$\alpha f(x)^2 = \frac{1}{|x|} < \frac{4}{r} < 1 = \alpha_0 \qquad \forall x \in D.$$

Finally, because $\rho \in [r, C\,\kappa^{-1}]$,

$$\Big|\frac{\delta}{|x|} - \kappa\Big| \leq \frac{2C+\delta}{|x|} = C_0 f(x)^2 \quad \text{ for all } x \in D.$$

The condition (6.43) is trivially fulfilled by the Coulomb potential $-\delta/|x|$ with our choice of f and l, and by the choice of f and l and the requirement (6.48), the condition (6.26) is also satisfied. In this way, all the conditions of Theorem 6.8 are fulfilled, and so

$$
\begin{aligned}
&\Bigg|\mathrm{Tr}\Big\{\,\psi\,\Big|\sqrt{p^2+1} - 1 - \frac{\delta}{|x|} - \kappa\Big|_-\Big\} \\
&\qquad\qquad\qquad - \frac{1}{(2\pi)^3}\iint d^3p\, d^3x \Big[\frac{p^2}{2} - \frac{\delta}{|x|} + \kappa\Big]_-\Bigg| \\
&\leq C\int_{|x|=\frac{r}{4}}^{2\rho} f(x)^3 l(x)^{-2}\, d^3x + C'\int_{|x|=\frac{r}{4}}^{2\rho} f(x)^{-2-N} l(x)^{-N-3}\, d^3x \\
&= \tilde{C}\int_{\frac{r}{4}}^{2\rho} t^{-3/2}\, dt + \int_{\frac{r}{4}}^{2\rho} t^{-N/2}\, dt \leq \tilde{C} r^{-1/2},
\end{aligned}
$$

by choosing $N = 3$. This proves the bound (6.49). $\square$

7. The Main Theorems

We are ready to prove the two main main theorems of this thesis; we start with:

Theorem 7.1. *Let $\phi \in C_0^\infty(\mathbb{R}^3)$ be a function such that $|\phi| \le 1$ and*

$$\phi(x) = \begin{cases} 1 & , \quad |x| \le 1 \\ 0 & , \quad |x| \ge 2 \end{cases}$$

and let $\phi_\rho(x) = \phi(x/\rho)$ for $\rho > 0$. Let

$$H_{rel} = \sqrt{-\Delta + 1} - 1 - \frac{\delta}{|x|}$$

for some $\delta < 2/\pi$ and let

$$\mathfrak{W}_{cl}(\phi_\rho) = \frac{1}{(2\pi)^3} \iint d^3x\, d^3p\ \phi_\rho(x) \left[\frac{p^2}{2} - \frac{\delta}{|x|}\right]_- .$$

Then there exists a number $F(\delta)$, independent of the function ϕ, such that

$$\mathrm{Tr}\{\phi_\rho |H_{rel}|_-\} - \mathfrak{W}_{cl}(\phi_\rho) = F(\delta) + o(1) \quad , \quad \rho \to \infty. \tag{7.1}$$

Remark 7.2. It it very important to notice that it is the Weyl-term corresponding to the non-relativistic operator,

$$H_{cl} = \frac{p^2}{2} - \frac{\delta}{|x|} \tag{7.2}$$

and not that of the relativistic operator from (7.1) that occurs in the theorem. The corresponding non-relativistic Weyl-term is not finite.

Proof. The aim is to show that

$$\left\{\mathfrak{A}_n\right\}_{n\in\mathbb{N}} = \left\{\mathrm{Tr}\{\phi_n |H_{rel}|_-\} - \mathfrak{W}_{cl}(\phi_n)\right\}_{n\in\mathbb{N}}$$

is a Cauchy-sequence. Note that since both $\mathrm{Tr}\{\phi_n|H_{rel}|_-\}$ and $\mathfrak{W}_{cl}(\phi_n)$ are finite, this will prove the theorem. The idea is to pass by the relativistic Weyl-term, away from the singularity of the Coulomb potential (where the divergence of this term occurs). Since

$$\mathfrak{A}_n - \mathfrak{A}_m = \mathrm{Tr}\{(\phi_n - \phi_m)|H_{rel}|_-\} - \mathfrak{W}_{cl}(\phi_n - \phi_m) \quad , \quad n \ge m \ge N$$

for some N very large, we are away from the singularity, and so the potential, and hence the momentum $|p|$, is small on the area of integration. This will allow us to relate $\mathfrak{W}_{cl}(\phi_n - \phi_m)$ and

$$\begin{aligned} &\mathfrak{W}_{rel}(\phi_n - \phi_m) \\ &= \frac{1}{(2\pi)^3} \iint d^3x\, d^3p\ \big(\phi_n(x) - \phi_m(x)\big) \left[\sqrt{p^2+1} - 1 - \frac{\delta}{|x|}\right]_-, \end{aligned}$$

and also, by the analysis in section 6, we will now be able to compare $\mathrm{Tr}\{(\phi_n - \phi_m)|H_{rel}|_-\}$ and $\mathfrak{W}_{rel}(\phi_n - \phi_m)$ since we are in an area where the potential is smooth.

More precisely, we start by proving the following lemma:

Lemma 7.3. *For $n \geq m \geq 2$:*

$$\left|\mathfrak{W}_{rel}(\phi_n - \phi_m) - \mathfrak{W}_{cl}(\phi_n - \phi_m)\right| \leq \frac{C}{\sqrt{m}}. \tag{7.3}$$

Proof. Note that (remember that $\sqrt{p^2+1} - 1 \leq p^2/2$)

$$\begin{aligned}
&\left|\mathfrak{W}_{rel}(\phi_n - \phi_m) - \mathfrak{W}_{cl}(\phi_n - \phi_m)\right| \\
&\leq \frac{1}{(2\pi)^3} \iint_A d^3x\, d^3p \Big(\Big[\sqrt{p^2+1} - 1 - \frac{\delta}{|x|}\Big]_- \\
&\qquad\qquad\qquad - \Big[\frac{p^2}{2} - \frac{\delta}{|x|}\Big]_- \Big) \\
&+ \frac{1}{(2\pi)^3} \iint_B d^3x\, d^3p \, \Big[\frac{\delta}{|x|} - \big(\sqrt{p^2+1} - 1\big)\Big]_+
\end{aligned}$$

where

$$A = \Big\{(x,p) \;\Big|\; \frac{p^2}{2} - \frac{\delta}{|x|} \leq 0\,,\; m \leq |x| \leq 2n\;\Big\}$$

and

$$\begin{aligned}
B &= \Big\{(x,p) \;\Big|\sqrt{p^2+1} - 1 - \frac{\delta}{|x|} \leq 0 \leq \frac{p^2}{2} - \frac{\delta}{|x|}\,, \\
&\qquad\qquad\qquad\qquad m \leq |x| \leq 2n \;\Big\} \\
&= \Big\{(x,p) \;\Big|\; \frac{2\delta}{|x|} \leq p^2 \leq \frac{2\delta}{|x|}\Big(1 + \frac{\delta}{2|x|}\Big)\,, m \leq |x| \leq 2n\;\Big\}.
\end{aligned}$$

Let us start by studying the integral over A:

$$\begin{aligned}
&\frac{1}{(2\pi)^3} \iint_A d^3x\, d^3p \Big(\Big[\sqrt{p^2+1} - 1 - \frac{\delta}{|x|}\Big]_- \\
&\qquad\qquad\qquad - \Big[\frac{p^2}{2} - \frac{\delta}{|x|}\Big]_- \Big) \\
&= \frac{1}{(2\pi)^3} \iint_A d^3x\, d^3p \Big[\frac{p^2}{2} - \sqrt{p^2+1} - 1\Big].
\end{aligned} \tag{7.4}$$

Now, by a Taylor expansion,

$$\begin{aligned}
&\sqrt{p^2+1} - 1 \\
&= \frac{p^2}{2} - \frac{p^4}{8} + \frac{1}{24}\int_0^{|p|} (|p| - t)^4 \frac{15t(3 - 4t^2)}{(1+t^2)^{9/2}}\, dt \geq \frac{p^2}{2} - \frac{p^4}{8}.
\end{aligned}$$

The inequality since on A:

$$|p| \leq \sqrt{\frac{2\delta}{m}} < \sqrt{\frac{2}{\pi}} < \frac{\sqrt{3}}{2},$$

and so the integrand is postive. In this way (7.4) is bounded by

$$\frac{1}{(2\pi)^2}\iint_A d^3x\, d^3p\, \left(\frac{p^4}{8}\right) = \frac{1}{4\pi}\int_m^{2n} |x|^2\, d|x| \int_0^{\sqrt{\frac{2\delta}{|x|}}} |p|^6\, d|p|$$
$$= \frac{4\sqrt{2}}{7\pi}\delta^{7/2}\left(\frac{1}{\sqrt{m}} - \frac{1}{\sqrt{2n}}\right) \le \frac{4\sqrt{2}}{7\pi}\delta^{7/2}\frac{1}{\sqrt{m}}. \tag{7.5}$$

As for the integral over B, dropping the kintetic energy $\sqrt{p^2+1}-1$, we get that

$$\frac{1}{(2\pi)^3}\iint_B d^3x\, d^3p\, \left[\frac{\delta}{|x|} - \left(\sqrt{p^2+1}-1\right)\right]_+$$
$$\le \frac{2}{\pi}\int_m^{2n} d|x| \left(|x|^2 \frac{\delta}{|x|}\int_{4Y}^{4Y(1+Y)} \frac{\sqrt{|p|^2}}{2}\, d(|p|^2)\right)$$
$$\le \frac{2\delta}{3\pi}\int_m^{2n} |x|\left(4Y\right)^{3/2}\left(\left(1+Y\right)^{3/2} - 1\right) d|x| \tag{7.6}$$

with $Y = \frac{\delta}{2|x|}$. Now, by a Taylor expansion around $y=0$,

$$(1+y)^{3/2} = 1 + \frac{3}{2}y + \frac{3}{8}y^2 - \frac{3}{16}\int_0^y (y-t)^2(1+t)^{-3/2}\, dt$$
$$\le 1 + \frac{3}{2}y + \frac{3}{8}y^2,$$

and so (7.6) is bounded by

$$\frac{4\sqrt{2}\delta^{5/2}}{3\pi}\int_m^{2n} |x|^{-1/2}\left(\frac{3}{2}\frac{\delta}{2|x|} + \frac{3}{8}\frac{\delta^2}{4|x|^2}\right) d|x|$$
$$= \frac{2\sqrt{2}\delta^{7/2}}{\pi}\left(\frac{1}{\sqrt{m}} - \frac{1}{\sqrt{2n}}\right) + \frac{2\sqrt{2}\delta^{9/2}}{24\pi}\left(\frac{1}{m\sqrt{m}} - \frac{1}{2n\sqrt{2n}}\right) \le \frac{C}{\sqrt{m}}. \tag{7.7}$$

Now the estimates (7.5) and (7.7) provide the bound (7.3). □

Using the lemma we get that for $n \ge m \ge 2$:

$$\left|\mathfrak{A}_n - \mathfrak{A}_m\right| \le \left|\mathrm{Tr}\{(\phi_n - \phi_m)|H_{rel}|_-\} - \mathfrak{W}_{rel}(\phi_n - \phi_m)\right|$$
$$+ \left|\mathfrak{W}_{rel}(\phi_n - \phi_m) - \mathfrak{W}_{cl}(\phi_n - \phi_m)\right|$$
$$\le \left|\mathrm{Tr}\{(\phi_n - \phi_m)|H_{rel}|_-\} - \mathfrak{W}_{rel}(\phi_n - \phi_m)\right| \quad + \frac{C}{\sqrt{m}}. \tag{7.8}$$

We now use Theorem 6.9 with $\kappa = 0$. To do this, note that the operator $A = H_{rel}$ satisfies Assumption 5.1 in the set $D = \left\{ x \mid \frac{m}{4} < |x| < 4n\right\}$. To see this, take

$$V(x) = -\chi(x)\,\frac{\delta}{|x|}$$

with $\chi \in C_0^\infty(\mathbb{R}^3 \setminus B(1/8))$, $\chi \equiv 1$ on D. Then (1) in Assumption 5.1 is satisfied due to Proposition B.20 and (2) due to the choice of V above. Finally $H_{rel} \geq -1$, see Herbst [14]. By construction, $\psi = \phi_n - \phi_m$ satisfies (6.48) on D and V above obviously satisfies (6.47). By Theorem 6.9 (with $\kappa = 0$) this means that

$$\Big|\mathrm{Tr}\{(\phi_n - \phi_m)|H_{rel}|_-\} - \mathfrak{W}_{rel}(\phi_n - \phi_m)\Big| \leq \frac{C}{\sqrt{m}}. \tag{7.9}$$

Together with (7.8) this showes that the sequence $\{\mathfrak{A}_n\}_{n\in\mathbb{N}}$ is Cauchy and hence convergent. This finishes the proof of the theorem. $\square$

Proof of Theorem 1.4. Using the unitary transformation $y = \alpha^{-1}x$ (and therefore $\Delta_y = \alpha^2\Delta_x$), Theorem 7.1 gives us (choosing $\rho = \alpha^{-\epsilon}$ for some $\epsilon > 0$ and with $\delta = \alpha Z$) that

$$\begin{aligned}
&\mathrm{Tr}\Big\{\phi_{\alpha^{1-\epsilon}}(x)\Big|\sqrt{-\alpha^{-2}\Delta_x + \alpha^{-4}} - \alpha^{-2} - \frac{Z}{|x|}\Big|_-\Big\} \\
&\quad = \alpha^{-2}\Big(\mathrm{Tr}\Big\{\phi_{\alpha^{-\epsilon}}(y)\Big|\sqrt{-\Delta_y + 1} - 1 + \frac{\delta}{|y|}\Big|_-\Big\}\Big) \\
&\quad = \alpha^{-2}\Big(\mathfrak{W}_{rel}(\phi_{\alpha^{-\epsilon}}) + F(\delta) + o(1)\Big) \quad , \quad \alpha \to 0 \\
&\quad = \frac{1}{(2\pi)^3}\iint d^3x\, d^3p\, \left(\phi_{Z^{-1+\epsilon}}(x)\right)\Big[\frac{p^2}{2} - \frac{\delta}{|x|}\Big]_- \\
&\qquad\qquad + \tilde{F}(\delta)Z^2 + o(Z^2) \quad , \quad Z \to \infty.
\end{aligned}$$

In the last equality we used the changes of variables, $x = \alpha y$ and $p = \alpha^{-1}q$ (here, $\tilde{F}(\delta) = F(\delta)/\delta^2$, since $\delta = \alpha Z$). This provides the prove of Theorem 1.4. $\square$

The other main theorem of this section gives a different way of describing the constant $F(\delta)$:

Theorem 7.4. *Let, for some $\delta < 2/\pi$*

$$H_{rel} = \sqrt{-\Delta + 1} - 1 - \frac{\delta}{|x|} \tag{7.10}$$

and let for $\kappa \in]0, 1]$,

$$\mathfrak{W}_{cl}(\kappa) = \frac{1}{(2\pi)^3}\iint d^3x\, d^3p\Big[\frac{p^2}{2} - \frac{\delta}{|x|} + \kappa\Big]_-.$$

Then, with $F(\delta)$ the constant from Theorem 7.1:

$$\lim_{\kappa\to 0}\Big[\mathrm{Tr}\{|H_{rel} + \kappa|_-\} - \mathfrak{W}_{cl}(\kappa)\Big] = F(\delta). \tag{7.11}$$

Remark 7.5. Note that $\mathfrak{W}_{cl}$ is now a function of the κ added to the Coulomb potential, and of the cut-off function ϕ_ρ. We write $\mathfrak{W}_{cl}(\phi \equiv 1, \kappa) = \mathfrak{W}_{cl}(\kappa)$.

Proof. We use the cut-off function from Theorem 7.1: Let $\phi \in C_0^\infty(\mathbb{R}^3)$ be a function such that $|\phi| \leq 1$ and

$$\phi(x) = \begin{cases} 1 & , \quad |x| \leq 1 \\ 0 & , \quad |x| \geq 2. \end{cases}$$

Let κ be fixed and choose $\rho \geq a\kappa^{-1}$ for some $a > 1+\delta$ and let $\phi_\rho(x) = \phi(x/\rho)$. For $r \in [32^2, \rho]$, split configuration space in three regions: an inner ball of radius r, a spherical shell with $r \leq |x| \leq \rho$ and an outer region, with $|x| \geq \rho$. Then $\mathrm{Tr}\{|H_{rel}+\kappa|_-\}$ and $\mathfrak{W}_{cl}(\kappa)$ split accordingly:

$$\begin{aligned} \mathrm{Tr}\{|H_{rel}+\kappa|_-\} &= \mathrm{Tr}\{\phi_r|H_{rel}+\kappa|_-\} + \mathrm{Tr}\{(\phi_\rho - \phi_r)|H_{rel}+\kappa|_-\} \\ &\quad + \mathrm{Tr}\{(1-\phi_\rho)|H_{rel}+\kappa|_-\}, \\ \mathfrak{W}_{cl}(1,\kappa) &= \mathfrak{W}_{cl}(\phi_r,\kappa) + \mathfrak{W}_{cl}((\phi_\rho-\phi_r),\kappa) \\ &\quad + \mathfrak{W}_{cl}((1-\phi_\rho),\kappa). \end{aligned} \tag{7.12}$$

We first note that with the choice of ρ as above, we have that

$$\mathfrak{W}_{cl}((1-\phi_\rho),\kappa) = 0. \tag{7.13}$$

This is because $\frac{\delta}{|x|} - \kappa \leq 0$ for $|x| \geq \rho$ and so

$$\big(1-\phi_\rho(x)\big)\Big[\frac{p^2}{2} - \frac{\delta}{|x|} + \kappa\Big]_- = 0 \qquad \forall (x,p).$$

Secondly we have, using Lemma E.1 (again, by our choice of ρ), that

$$\mathrm{Tr}\{(1-\phi_\rho)|H_{rel}+\kappa|_-\} \leq C\sqrt{\kappa}. \tag{7.14}$$

The restriction $\delta < 2/\pi$ comes about from this lemma. As for the term related to the shell $r \leq |x| \leq \rho$, we use Theorem 6.9 as in the proof of Theorem 7.1, this time with $\kappa \neq 0$. This gives (passing by the relativistic Weyl-term $\mathfrak{W}_{rel}$ as in the proof of Theorem 7.1), that

$$\Big|\mathrm{Tr}\{(\phi_\rho-\phi_r)|H_{rel}+\kappa|_-\} - \mathfrak{W}_{cl}((\phi_\rho-\phi_r),\kappa)\Big| \leq \frac{C}{\sqrt{r}}. \tag{7.15}$$

We are left with the terms for the ball $B(2r)$. We re-write the difference between them as

$$\begin{aligned} \mathrm{Tr}\{\phi_r|H_{rel}+\kappa|_-\} - \mathfrak{W}_{cl}(\phi_r,\kappa) &= \mathrm{Tr}\{\phi_r|H_{rel}+\kappa|_-\} - \mathrm{Tr}\{\phi_r|H_{rel}|_-\} \\ &\quad + \mathrm{Tr}\{\phi_r|H_{rel}|_-\} - \mathfrak{W}_{cl}(\phi_r,0) \\ &\quad + \mathfrak{W}_{cl}(\phi_r,0) - \mathfrak{W}_{cl}(\phi_r,\kappa). \end{aligned} \tag{7.16}$$

We immidiately note, that the second term tends to the constant $F(\delta)$ from Theorem 7.1 as $r \to \infty$. Next, we have that

$$\lim_{\kappa\to 0}\Big|\mathfrak{W}_{cl}(\phi_r,0) - \mathfrak{W}_{cl}(\phi_r,\kappa)\Big| = 0 \qquad \forall r, \tag{7.17}$$

since, for r fixed,

$$\Big|\mathfrak{W}_{cl}(\phi_r,0)-\mathfrak{W}_{cl}(\phi_r,\kappa)\Big| \le \frac{1}{(2\pi)^3}\iint_E d^3x\, d^3p\ \kappa + \frac{1}{(2\pi)^3}\iint_F d^3x\, d^3p\ \left[\frac{\delta}{|x|}-\frac{p^2}{2}\right]_+$$

with

$$E=\Big\{(x,p)\ \Big|\ p^2\le \frac{2\delta}{|x|}-2\kappa\ ,\ |x|\le 2r\Big\}$$

and

$$F=\Big\{(x,p)\ \Big|\ \frac{2\delta}{|x|}-2\kappa\le p^2\le \frac{2\delta}{|x|}\ ,\ |x|\le 2r\Big\}$$

Now,

$$\frac{1}{(2\pi)^3}\iint_E d^3x\, d^3p\ \kappa \le \frac{32\delta^{3/2}}{3\pi} r^{3/2}\kappa$$

and

$$\begin{aligned}\frac{1}{(2\pi)^3}\iint_F & d^3x\, d^3p\ \left[\frac{\delta}{|x|}-\frac{p^2}{2}\right]_+ \\ &= \frac{2}{3\pi}\int_0^{2r} d|x|\ \left[\ |x|^2\left(\frac{\delta}{|x|}-\kappa\right)\left(\frac{2\delta}{|x|}\right)^{3/2}\left\{1-\left(1-\frac{\kappa|x|}{\delta}\right)^{3/2}\right\}\right] \\ &\le \frac{8\delta^{3/2}}{3\pi} r^{3/2}\kappa\end{aligned}$$

by the Taylor expansion

$$(1-x)^{3/2}=1-\frac{3}{2}x+\frac{3}{8}\int_0^x (x-t)(1-t)^{-1/2}\,dt \ge 1-\frac{3}{2}x.$$

This proves (7.17).

Finally the term

$$\mathrm{Tr}\{\phi_r|H_{rel}+\kappa|_-\}-\mathrm{Tr}\{\phi_r|H_{rel}|_-\}.$$

We note that the potentials $V=-\frac{\delta}{|x|}$ and $V_\kappa=V+\kappa$ can be written in the form (C.4):

$$\left.\begin{aligned} V(x) &= Y(x)\Psi(x)Y(x) \\ V_\kappa(x) &= Y(x)(\Psi(x)+F(x))Y(x)\end{aligned}\right\}\quad \text{for } x\in\mathbb{R}^3$$

with

$$\Psi(x)=-\delta\quad ,\quad Y(x)=|x|^{-1/2}\quad ,\quad F(x)=\kappa|x|.$$

We need to note that Y satisfies

$$\|Yu\|^2\le \varepsilon(H_0u,u)+\|u\|^2 \quad \text{for all } u\in C_0^\infty(\mathbb{R}^3)$$

with $H_0=\sqrt{-\Delta+1}-1$, since $H_0-\frac{\delta}{|x|}\ge 0$ as a quadratic form as long as $\delta\le 2/\pi$, see Herbst [14, Theorem 2.1]. This means that we can apply Theorem C.6 with $\alpha = \beta \equiv 1$ and $s = 1$. This gives us that for any fixed $L_0 > 0$ we have, for all $l \geq r$, $L \geq L_0$ and $K > 3$:

$$\Big|\mathrm{Tr}\{\phi_r|H_{rel} + \kappa|_-\} - \mathrm{Tr}\{\phi_r|H_{rel}|_-\}\Big| \\ \leq C_K L^{2K+1} l^3 \big(l^{-2K} + \kappa l\big) + C'_K L^{-1} r^3 \tag{7.18}$$

since the quantity $K(0, r)$ defined in (C.8) is merely κl (remember that $r \geq 32^2$; in Theorem C.6 the length l was called ρ).

We now summarize: By the decompositions in (7.12) and (7.16) and the results (7.13), (7.14) and (7.17) we have, for any $l \geq r$ and $L \geq L_0$, that

$$\lim_{\kappa \to 0} \Big|\mathrm{Tr}\{|H_{rel} + \kappa|_-\} - \mathfrak{W}_{cl}(\kappa) - F(\delta)\Big| \\ \leq \Big|\mathrm{Tr}\{\phi_r|H_{rel}|_-\} - \mathfrak{W}_{cl}(\phi_r, 0) - F(\delta)\Big| \\ + \frac{C}{\sqrt{r}} + C_K L^{2K+1} l^{3-2K} + C'_K L^{-1} r^3. \tag{7.19}$$

Choosing now $L = r^{3+\varepsilon}$ and $l = L^{1+\varepsilon}$ and K sufficiently large, Theorem 7.1 gives us that the right hand side in (7.19) tends to zero as we let r tend to infinity. This proves the theorem. $\square$

Proof of Theorem 1.6. Let $g(Z)$ be any function with $g(Z) = o(Z^2)$ (such that $\alpha^2 g(Z) \to 0$ as $\alpha \to 0$, with $\delta = \alpha Z$ fixed). Then Theorem 7.4 gives us, again using the unitary transformation $y = \alpha^{-1} x$, that

$$\lim_{Z\to\infty} Z^{-2}\Big|\mathrm{Tr}\Big\{\big|\sqrt{-\alpha^{-2}\Delta_x + \alpha^{-4}} - \alpha^{-2} - \frac{Z}{|x|} + g(Z)\,\big|_-\Big\} \\ - \frac{1}{(2\pi)^3}\iint d^3x\, d^3p\,\Big[\frac{p^2}{2} - \frac{\delta}{|x|} + g(Z)\Big]_- - \tilde{F}(\delta) Z^2\,\Big| \\ = \lim_{\alpha\to 0}\Big|\mathrm{Tr}\Big\{\big|\sqrt{-\Delta_y + 1} - 1 + \frac{\delta}{|y|} + \alpha^2 g(Z)\big|_-\Big\} \\ - \frac{1}{(2\pi)^3}\iint d^3y\, d^3q\Big[\frac{q^2}{2} - \frac{\delta}{|y|} + \alpha^2 g(Z)\Big]_- - F(\delta)\Big| = 0.$$

This proves Theorem 1.6. $\square$

Appendix A. Semi-classical Analysis

In this appendix we will be citing results about the semi-classical analysis of pseudo-differential operators (ΨDO's) needed for our study of the relativistic Herbst-operator. We refer to Robert [26] for the general theory of so-called '$h - \Psi$DO' and to Sobolev [38] for the results of more specific relevans for our purposes (see also Helffer and Robert [13] and Sobolev [37]). The idea of this appendix is to provide a result on the trace of a certain class of operators — to leading order in some parameter, this will be given by the appropriate semi-classical integral, the so-called 'Weyl-term'. This result has a certain uniformity in the symbol of the operator which we will take advantage of.

We start by some general set-up, for which we refer to the literature mentioned above. Results will be stated for general dimension n, though we shall only be interested in the case $n = 3$.

Definition A.1. A 'temperate weight in $\mathbb{R}^n$' is a continuous function $\rho : \mathbb{R}^n \to [0, \infty[$, for which there exist $C_0 > 0$ and $N_0 > 0$ such that

$$\rho(x) \leq C_0\, \rho(x_1)\big(1 + |x - x_1|\big)^{N_0} \quad \text{for all } x, x_1 \in \mathbb{R}^n.$$

Weights are used to measure the decay of symbols for ΨDO's, in the following sense:

Definition A.2. Let $\Omega \subset \mathbb{R}^{2n} = \mathbb{R}^n_x \times \mathbb{R}^n_\xi$ be an open set and let ρ be a temperate weight in $\mathbb{R}^{2n}$. We say, that 'a is a symbol in Ω with weight ρ' if $a \in C^\infty(\Omega)$ and if a satisfies

$$|\partial_x^\gamma \partial_\xi^\eta a(x,\xi)| \leq C_{\gamma,\eta}\, \rho(x,\xi) \quad \text{for all } (x,\xi) \in \Omega \text{ and } \gamma, \eta \in \mathbb{N}^n. \tag{A.1}$$

This definition ensures that the iterated integral in the following definition converges:

Definition A.3. For a Weyl-symbol a in $\mathbb{R}^n_x \times \mathbb{R}^n_\xi$ in the above sense and $h \in\,]0, h_0]$ for some $h_0 > 0$ fixed, we define the operator $A = \mathrm{op}^w_h a$ by

$$\begin{aligned}(Au)(x) &= \frac{1}{(2\pi)^n} \iint e^{i(x-y)p} a\big(\tfrac{x+y}{2}, hp; h\big) u(y)\, d^n y\, d^n p \\ &= \frac{1}{(2\pi h)^n} \iint e^{\frac{i}{h}(x-y)\xi} a\big(\tfrac{x+y}{2}, \xi; h\big) u(y)\, d^n y\, d^n \xi. \end{aligned} \tag{A.2}$$

We denote such operators by '$h-$pseudo-differential operators' ($h-$ ΨDO's).

First two criteria on the weight-function ρ that allow one to conclude properties of the operator $A = \mathrm{op}^w_h a$:

Proposition A.4.

(*1*) *If the weight function ρ in (A.1) is bounded, then the operator A defined by (A.2) is a bounded operator, and*

$$\|A\| \leq C_n \sup_{|\gamma| \leq k(n), |\eta| \leq k(n)} h^{|\eta|} |\partial_x^\gamma \partial_\xi^\eta a(x,\xi)|, \tag{A.3}$$

with constants C_n and $k(n)$ that only depend on the dimension n.

(*2*) *If $\rho \in L^1(\mathbb{R}^n_x \times \mathbb{R}^n_\xi)$, then $A \in \mathfrak{S}_1$ (the trace class operators), and*

$$\|A\|_1 \leq C'_n\, h^{-n} \sum_{|\gamma|+|\eta| \leq 2n+2} h^{|\eta|} \int |\partial_x^\gamma \partial_\xi^\eta a(x,\xi)|\, d^n x\, d^n \xi, \tag{A.4}$$

where C'_n only depends on the dimension n.

Next, it will be important to be able to compute the symbol of the composition of $h-\Psi$DO's: For two symbols a_1 and a_2 in $\mathcal{B}^\infty(\mathbb{R}^n_x \times \mathbb{R}^n_\xi)$, there exists a unique Weyl symbol $a \in \mathcal{B}^\infty(\mathbb{R}^n_x \times \mathbb{R}^n_\xi)$ such that $\mathrm{op}^w_h a_1\ \mathrm{op}^w_h a_2 = \mathrm{op}^w_h a$; this symbol satisfies the expansion:

$$\begin{aligned} & a(x,\xi) \\ & = \sum_{l=0}^{N} (-i)^l h^l \sum_{|\gamma|+|\eta|=l} \frac{1}{\gamma!\eta!} \left(\frac{1}{2}\right)^{|\gamma|} \left(-\frac{1}{2}\right)^{|\eta|} \partial_x^\eta \partial_\xi^\gamma a_1(x,\xi) \partial_x^\gamma \partial_\xi^\eta a_2(x,\xi) \\ & \quad + h^{N+1} r_{N+1}(x,\xi;h) \quad , \\ & \qquad r_{N+1}(\,\cdot\,,\,\cdot\,;h) \in \mathcal{B}^\infty(\mathbb{R}^n_x \times (\mathbb{R}^n_\xi) \quad , \quad \forall N > 0. \end{aligned} \tag{A.5}$$

By Proposition A.4 the operator $R_{N+1}(h) = \mathrm{op}^w_h r_{N+1}$ is bounded, by a constant uniform in the symbols a_1 and a_2 in the sense that it only depends on the constants in their respective weight estimates (A.1).

Furthermore, suppose one of the symbols a_1 or a_2 is supported in the ball $B_{x,\xi}(E)$, for some $E > 0$. Then

$$\|R_{N+1}(h)\|_1 \le C\, h^{-n} \quad , \quad C = C(E). \tag{A.6}$$

From the expansion (A.5) follows the next lemma:

Lemma A.5. *Let $a_1, a_2 \in \mathcal{B}^\infty(\mathbb{R}^n_x \times \mathbb{R}^n_\xi)$ and*

$$a_1(x,\xi) = 0 \quad , \quad (x,\xi) \in \operatorname{supp} a_2.$$

Then

$$\|\mathrm{op}^w_h a_1\ \mathrm{op}^w_h a_2\| \le C_N\, h^N \quad , \quad \forall N > 0. \tag{A.7}$$

If furthermore $a_2 \in C_0^\infty(B_{x,\xi}(E))$ for some $E > 0$, then

$$\|\mathrm{op}^w_h a_1\ \mathrm{op}^w_h a_2\|_1 \le \tilde{C}_N\, h^N \quad , \quad \forall N > 0. \tag{A.8}$$

The constants $\tilde{C}_N$ in (A.8) depend on the number E.

The next result will be the asymptotic expansion in powers of h for a C_0^∞- function of an $h-\Psi$DO, by the calculus due to Helffer and Robert [13]:

Theorem A.6. *Given a symbol $a(x,\xi;h)$, real and bounded from below, then the operator $A = \mathrm{op}^w_h a$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$. Assume additionally that $a(x,\xi;h) = a(x,\xi)$ is independent of h and that there exist positive numbers, b and c, such that $a+b$ is a temperate weight, $a(x,p)+b \ge c$ and a is a symbol of weight $a+b$. Then for $g \in C_0^\infty(\mathbb{R})$ and any integer $N > 0$ we have the expansion*

$$g(A) = \sum_{j=0}^{N} h^j \mathrm{op}^w_h a_{g,j} + h^{N+1} R_{g,N+1}(h) \tag{A.9}$$

with $\|R_{g,N+1}(h)\| \leq C_N$, *independently of* h, *and the symbols* $a_{g,j}$ *given by*

$$\begin{aligned} a_{g,0}(x,\xi) &= g(a(x,\xi)), \\ a_{g,1}(x,\xi) &= 0, \\ a_{g,j}(x,\xi) &= \sum_{k=1}^{2j-1} \frac{(-1)^k}{k!}\, d_{j,k}\, \partial_\lambda^k g(a(x,\xi)) \quad , \quad j \geq 2. \end{aligned}$$

The coefficients $d_{j,k}$ *are universal polynomials of* $\partial_x^{m_1}\partial_\xi^{m_2} a$, $m_1 + m_2 \leq j$.

Remark A.7. Note, that if $\{a_t\}_t$ is a family of symbols as above, such that $a_t + b$ is a weight, $a_t + b \geq c$ and a_t is a symbol of weight $a_t + b$, all uniformly in the variable t (including the constants in (A.1)), then the expansion above is uniform in t, in the sense that the constants C_N in the estimates $\|R_{g,N+1}(h)\| \leq C_N$ do not depend on t. All results in this appendix will be 'uniform in the symbol' in this sense. (See Sobolev [37, Ch. 5, p. 361]). This fact will be crucial for our application of the results in this appendix.

In the following, we will assume A to be an $h - \Psi$DO with a real-valued symbol, bounded from below, so that A is essentially self-adjoint, according to Theorem A.6. We also need an $h - \Psi$DO $\Theta = \mathrm{op}_h^w(\theta)$, with a real-valued symbol

$$\theta \in C_0^\infty\big(B_x(E) \times B_\xi(R)\big), \quad E > 0, \quad R > 0. \tag{A.10}$$

Think of this as a cut-off in phase-space.

What we will be discussing here is the $h -$ asymptotics of the trace

$$\mathrm{Tr}\{\Theta\, g(A)\}$$

for some bounded function g; the finiteness of this quantity is ensured by the fact that $\|\Theta\|_1 < \infty$ by Proposition A.4.

When studying semi-classical asymptotics for traces of functions of $h - \Psi$DO's, one starts by studying the propagator

$$U_h(t; A) = \exp\{\frac{i}{h} At\},$$

and then uses the representation

$$g(A) = \frac{1}{h\sqrt{2\pi}} \int \hat{g}(t) U_h(t; A)\, dt.$$

where $\hat{g}(t)$ is the $h -$ Fourier transform of g,

$$\hat{g}(t) = \frac{1}{\sqrt{2\pi}} \int g(\lambda) e^{it\lambda/h}\, d\lambda.$$

Then one approximates the propagator of the time evolution $U_h(t; A)$ by an $h-$ Fourier integral operator ($h-$ FIO) $G_h(t)$, having the kernel

$$\mathcal{G}(x, y, t) = (2\pi h)^{-n} \int e^{\frac{i}{h}(S(x,\xi,t)-y\cdot\xi)} v(x, \xi, t; h)\, d^n\xi. \tag{A.11}$$

Here, the phase $S(x, \xi, t)$ is real-valued and the amplitude v is of the form

$$v(x, \xi, t; h) = \sum_{j=0}^{N} h^j\, v_j(x, \xi, t)$$

with compactly supported functions $v_j(\cdot, \cdot, t)$. We suppose also that at time $t = 0$ the operator is close to the identity in the following sense:

$$G_h(0) = \Phi = \mathrm{op}_h^w \phi \tag{A.12}$$

with a real-valued function ϕ such that

$$\phi \in C_0^\infty(B_x(2E) \times B_\xi(2R))$$

and

$$\phi(x, \xi) = 1 \ \text{ for } \ (x, \xi) \in B_x(3E/2) \times B_\xi(3R/2).$$

To ensure the initial condition (A.12), we have to assume that

$$\begin{aligned} S(x, \xi, 0) &= x \cdot \xi \\ v_j(x, \xi, 0) &= 0, \quad j \geq 1. \end{aligned}$$

This will not be used in the sequel though, all we need is the following fact:

Proposition A.8. *There exist a number $T_0 > 0$ and functions*

$$S, v_j \in C^\infty\big(B_x(3E) \times B_\xi(3R) \times [-T_0, T_0]\big)$$

such that for any integer $N > 0$

$$\max_{|t| \leq T_0} \| - ih\partial_t G_h(t) + A\, G_h(t)\| \leq C_N h^{N+1}.$$

This says that the Fourier integral operator G_h approximates the time-evolution $U_h(t; A)$, in the sense that $U_h(t; A)$ satisfies the differential equation

$$-ih\partial_t U_h(t; A) + A\, U_h(t; A) = 0$$

whereas the term

$$-ih\partial_t G_h(t) + A\, G_h(t)$$

is small, in operator norm, to all orders of h, uniformly in the time $|t| \leq T_0$.

To continue, we fix some notation that will needed more generally than just in this chapter.

Let $T \in]0, T_0]$, where T_0 is the number (the 'time') from Proposition A.8, and let $\hat{\chi} \in C_0^\infty(-T, T)$ be a real-valued function such that

$$\begin{aligned} \hat{\chi}(t) &= \hat{\chi}(-t) \qquad \forall t, \\ \hat{\chi}(t) &= \frac{1}{\sqrt{2\pi}} \quad , \quad |t| \leq T/2. \end{aligned}$$

Then define

$$\chi_1(\tau) = \frac{1}{\sqrt{2\pi}} \int \hat{\chi}(t) e^{i\tau t}\, dt. \tag{A.13}$$

By (if necessary) replacing $\hat{\chi}$ with $\hat{\chi} * \hat{\chi}$ and assuming $\hat{\chi} > 0$, we can assume, that $\chi_1 \geq 0$ and that there exists a $T_1 \in]0, T[$, such that $\chi_1(\tau) \geq c > 0$ for $|\tau| \leq T_1$.

Define now the $h -$ scaled version of χ_1:

$$\chi_h(\tau) = \frac{1}{h} \chi_1\Big(\frac{\tau}{h}\Big). \tag{A.14}$$

Next, define for an integrable function $g \in L^1(\mathbb{R}^n)$ its by χ_h smoothed out version:

$$\begin{aligned} g^{(h)}(\tau) &= \big(g * \chi_h\big)(\tau) \\ &= \int g(\tau - \nu)\chi_h(\nu)\, d\nu = \int g(\nu)\chi_h(\tau - \nu)\, d\nu. \end{aligned} \tag{A.15}$$

We remark right away that

$$|g^{(h)}(\tau)| \leq \max_\nu \chi_h(\nu) \|g\|_{L^1} \leq C\, h^{-1}. \tag{A.16}$$

In order to say anything about the $h -$ asymptotics of the trace $\mathrm{Tr}\{\Theta\, g(A)\}$ one needs to assume a 'non-critical' condition on the gradient of the symbol on the 'energy-shell' $\{a(x, \xi) = \lambda\}$:

Assumption A.9. On the set

$$\Lambda(\lambda, \theta) = \{(x, \xi) \mid a(x, \xi) = \lambda,\ (x, \xi) \in \operatorname{supp} \theta\}$$

we have the lower bound

$$|\nabla a(x, \xi)| \geq \delta > 0. \tag{A.17}$$

We say that the value λ is a non-critical (critical) value of the operator A on the support of the function θ if Assumption A.9 is (not) satisfied. For a given energy λ we will denote the whole 'energy-shell', $\Lambda(\lambda, 1)$, by $\Lambda(\lambda)$.

This defined, we can finally formulate the following result on the $h -$ asymptotics of the trace $\mathrm{Tr}\{\Theta\, g(A)\}$ for various kinds of functions g:

Proposition A.10. *Let A be an $h-\Psi DO$ with a real-valued symbol $a = a(x,\xi)$ which is bounded from below, so that A is essentially self-adjoint (see Theorem A.6). Let $\Theta = \mathrm{op}_h^w(\theta)$ with some real-valued symbol*

$$\theta \in C_0^\infty\big(B_x(E) \times B_\xi(R)\big), \quad E > 0, \quad R > 0.$$

(*1*) *If $g \in C_0^\infty(\mathbb{R})$ then*

$$\mathrm{Tr}\{\Theta\, g(A)\} = \frac{1}{(2\pi h)^n} \int \theta(x,\xi) g(a(x,\xi))\, d^n x\, d^n \xi + C\, h^{2-n}. \tag{A.18}$$

(*2*) *Assume that Assumption A.9 is satisfied for some λ, with $|\lambda| \le \lambda_0$ for some fixed λ_0. Then*

$$\|\Theta\, \chi_h\big(A-\lambda\big)\|_1 \le C\, h^{-n}. \tag{A.19}$$

The constant C is uniform in λ, $|\lambda| \le \lambda_0$. Here, $\chi_h\big(A-\lambda\big)$ is the operator obtained from the spectral theorem by applying the function χ_h to the self-adjoint operator $A-\lambda$.

(*3*) *Let $g \in L^1(\mathbb{R}^n)$ be compactly supported, and assume that Assumption A.9 is satisfied for all $\lambda \in \mathrm{supp}\, g$. Then*

$$\mathrm{Tr}\{\Theta\, g^{(h)}(A)\} = \frac{1}{(2\pi h)^n} \int \theta(x,\xi) g(a(x,\xi))\, d^n x\, d^n \xi + C\, h^{2-n}. \tag{A.20}$$

Observe that the last result, (A.20), in Proposition A.10 gives the asymptotics of the trace related to $g^{(h)}$, the smoothed out version of the function g, as an integral related to the function g itself. To obtain the asymptotics of the trace related to the function g itself, we need what is known as a 'Tauberian argument' (see Rudin [27, p. 226]). Before that, we specify the class of functions we will be dealing with:

Definition A.11. A function $g \in C^\infty(\mathbb{R}\setminus\{0\})$ is said to belong to the class $C^{\infty,s}(\mathbb{R})$ for $s \in [0,1]$ if:

(*1*) $g \in C(\mathbb{R})$, $s > 0$.

(*2*) For some $r > 0$ and some C:

$$\begin{aligned} g(\lambda) &= 0, & &\lambda \ge C \\ |\partial_\lambda^m g(\lambda)| &\le C_m |\lambda|^r, & &\lambda \le -C, \quad \forall m \ge 0. \end{aligned}$$

(*3*) For $|\lambda| \le C$, $\lambda \ne 0$, and $m \ge 0$:

$$\begin{aligned} |\partial_\lambda^m g(\lambda)| &\le C_m |\lambda|^{s-m}, & &0 < s < 1 \\ |\partial_\lambda^m g(\lambda)| &\le C_m, & &s = 0,1. \end{aligned}$$

A function g is said to belong to $C_0^{\infty,s}(\mathbb{R})$, $s \in [0,1]$, if g is of compact support and $g \in C^{\infty,s}(\mathbb{R})$.

Define for $s \in [0,1]$ the functions

$$g_s(\lambda) = \begin{cases} |\lambda|^s, & \lambda \le 0 \\ 0, & \lambda > 0. \end{cases}$$

Note, that $g_s \in C^{\infty,s}(\mathbb{R})$. We will mainly be interested in g_s for $s = 1$, in order to study the sum of the negative eigenvalues of an operator.

We are ready to state the last result needed from this theory, namely on how, from information of the trace $\mathrm{Tr}\{\psi\, g^{(h)}(A)\}$ related to the (by the function χ_h) smoothed out version of g, to retrieve information on the trace $\mathrm{Tr}\{\psi\, g(A)\}$ related to g itself:

Proposition A.12. *Let A be a self adjoint operator, and let the function g belong to $C_0^{\infty,s}(\mathbb{R})$ for some $s \in [0,1]$.*

Let the function χ_1 be as defined above (see around (A.13)). Assume that for an operator $B \in \mathfrak{S}_2$ (the Hilbert-Schmidt operators), some positive function $Z(h)$ and some positive number $\delta > 0$, we have the estimate

$$\sup_{\lambda \in \mathcal{F}(\delta)} \|B^* \chi_h(A-\lambda)B\|_1 \le Z(h), \tag{A.21}$$

where

$$\mathcal{F}(\delta) = \{\lambda \in \mathbb{R} \,|\, \mathrm{dist}\{\mathrm{supp}\, g, \lambda\} \le \delta\,\}. \tag{A.22}$$

(See (A.14) and (A.19) for $\chi_h(A-\lambda)$).
Then, for all $N_1 > 0$:

$$\|B^*\big(g(A) - g^{(h)}(A)\big)B^*\|_1 \le C\, h^{1+s} Z(h) \quad + \quad C_{N_1} h^{N_1} \|B^* B\|_1. \tag{A.23}$$

Here, $g^{(h)} = g * \chi_h$, see (A.15). The constants C and C_{N_1} depend only on the number δ and the functions g and χ_1.

As mentioned earlier, we refer the reader to Robert [26], Helffer and Robert [13], and Sobolev [37, 38] for proofs of all the statements in this appendix. Here we only emphasize that all the above results are uniform in the sense stated in remark A.7, which will be essential for our use of these.

Appendix B. Estimate on Resolvents

Throughout this appendix, H and H_0 will denote the relativistic operators

$$H_0 = \sqrt{-\alpha^{-1}\beta^2\Delta + \alpha^{-2}} - \alpha^{-1} \quad , \quad H = H_0 + V. \tag{B.1}$$

We will also write $H_0 = \sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1}$ (with $p = -i\beta\nabla$) for convenience. Also, when we deal with the non-relativistic kinetic energy, $-\beta^2\Delta$, we will often denote this p^2. We emphasize again, that the 'classical' (non-relativistic) operator will never be denoted H.

By A we denote an abstract operator, which is equal to H in an open set $D \subset \mathbb{R}^3$ in the following sense:

Assumption B.1.
A is selfadjoint in $L^2(\mathbb{R}^3)$, semi-bounded from below and for any $\zeta \in C_0^\infty(D)$ the following holds:

(1) $\forall u \in \mathcal{D}[A]$ we have $u\zeta \in \mathcal{D}[A]$. $\exists \zeta_1 \in C_0^\infty(D)$ (depending on ζ) such that $\zeta_1\zeta = \zeta$ and

$$A[u, \zeta v] = A[\zeta_1 u, \zeta v] + \big(B\, u, v\big) \quad \forall u, v \in \mathcal{D}[A],$$

with an operator B satisfying

$$\|B\|_1 \leq C_{N,D,\zeta_1} \, \big(\sqrt{\alpha}\beta\big)^N \qquad \text{for all } N \in \mathbb{N}. \tag{B.2}$$

If D is a ball of radius $\rho \geq \rho_0$ for some $\rho_0 > 0$ fixed, then

$$\|B\|_1 \leq C_{N,\zeta_1} \left(\frac{\sqrt{\alpha}\beta}{\rho}\right)^N \qquad \text{for all } N \in \mathbb{N}. \tag{B.3}$$

(2) $\exists\, V$, real valued, with $X = |V|^{1/2}$ satisfying

$$\|Xu\|^2 \leq \varepsilon\big(H_0 u, u\big) + M(\beta, \alpha, \varepsilon)\|u\|^2 \quad \forall u \in C_0^\infty(\mathbb{R}^3) \tag{B.4}$$

for some $\varepsilon \in]0, 1[$, $M(\beta, \alpha, \varepsilon) \geq 1$ such that for all $v \in \mathcal{D}[A], u \in \mathcal{D}[H]$ we have $\zeta u \in \mathcal{D}[A], \zeta v \in \mathcal{D}[H]$ and

$$A[\zeta u, \zeta v] = H[\zeta u, \zeta v]$$

and

$$A\psi = H\psi \qquad \text{for all } \psi \in C_0^\infty(D). \tag{B.5}$$

(3) The operator A satisfies the lower bound $A \geq \alpha^{-1}$.

Here, $\mathcal{D}[A]$ is the form domain of the operator A. In particular, we note, that we only deal with potentials that are form bounded relatively to H_0, with a relative bound less than or equal to 1.

The first aim is to show that, for certain purposes, A and H are not too different. The idea being, that for certain properties of H, its actual behaviour outside the domain D is inessential in that we can use the operator A instead (modulo errors in powers of β), which only needs to coincide with H on D.

To this end, we study resolvents $R(z, H)$ of the pseudo-differential operator H. We assume that V is as in (2) above—this implies, that the operator $H = H_0 + V$ is well defined in the form sense, and gives rise to a self adjoint operator by taking the Friedrichs extension; by abuse of notation, we also shall denote this operator by H. From (2) it follows, that this operator satisfies

$$\inf \sigma(H) \geq -M(\beta, \alpha, \varepsilon) \equiv -M.$$

That is, $\sigma(H) \subset [-M, \infty)$; define $d_M(z) = \operatorname{dist}\{z, [-M, \infty)\}$.

Let χ and ϕ be functions with separated supports, more specifically, for some $\rho_0 > 0$ fixed, satisfying

$$\begin{aligned} \operatorname{supp}\chi \subset B(\rho), &\qquad 0 \le |\chi| \le 1 \\ \operatorname{supp}\phi \subset \mathbb{R}^3 \setminus B(\nu\rho), &\qquad 0 \le |\phi| \le 1 \end{aligned} \tag{B.6}$$

for some $\rho \ge \rho_0$ and $\nu > 1$. Note, that we do not assume anything on the regularity of either χ or ϕ.

These two functions shall be fixed throughout this appendix; the aim is to obtain estimates on various operators—in various norms—in powers of α, β and ρ.

Lemma B.2. *Let n, k be such that $n > 3$ and $k \le 2n$. For $p = \frac{2n}{k}$ we have, for all $N \ge 1$ and all $P \ge 1$:*

$$\begin{aligned} \|\chi\, R(z,H)\, \phi\|_p \le C\, &\frac{1}{d_M(z)} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^{\frac{3}{p}} \left(\frac{\beta}{\rho}\right)^{kN} \\ &\times \left\{ \left(\frac{(\,|z| + M\,)^{1/2}}{d_M(z)}\right)^{kN} + \frac{\alpha^P}{d_M(z)} \right\} \end{aligned} \tag{B.7}$$

In particular, for all $K > 3$, we have

$$\begin{aligned} \|\chi\, R(z,H)\, \phi\|_1 \le C\, &\frac{1}{d_M(z)} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^{3} \left(\frac{\beta}{\rho}\right)^{2K} \\ &\times \left\{ \left(\frac{(\,|z| + M\,)^{1/2}}{d_M(z)}\right)^{2K} + \frac{\alpha^P}{d_M(z)} \right\} \end{aligned} \tag{B.8}$$

Also, for all $N \ge 1$ we have

$$\begin{aligned} \|\chi\, R(z,H)\, \phi\| \le C\, &\frac{1}{d_M(z)} \left(\frac{\beta}{\rho}\right)^{N} \\ &\times \left\{ \left(\frac{(\,|z| + M\,)^{1/2}}{d_M(z)}\right)^{N} + \frac{\alpha^P}{d_M(z)} \right\} \end{aligned} \tag{B.9}$$

Proof. We first prove (B.8) from (B.7): Choose $N = 1$ and $k = 2n = 2K > 6$, then $p = 1$ and $Nk = 2K$.

Next, notice, that we only need to prove (B.7) for $N = 1$: assume namely that it holds for $N = 1$, then for general N, $\frac{2nN}{kN} = \frac{2n}{k}$ and so

$$\begin{aligned} &\|\chi R(z,H)\phi\|_{\frac{2n}{k}} = \|\chi R(z,H)\phi\|_{\frac{2nN}{kN}} \\ &\le C\, \frac{1}{d_M(z)} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^{\frac{3kN}{2nN}} \left(\frac{\beta}{\rho}\right)^{kN} \left\{ \left(\frac{(\,|z| + M\,)^{1/2}}{d_M(z)}\right)^{kN} + \frac{\alpha^P}{d_M(z)} \right\} \\ &= C\, \frac{1}{d_M(z)} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^{\frac{3k}{2n}} \left(\frac{\beta}{\rho}\right)^{kN} \left\{ \left(\frac{(\,|z| + M\,)^{1/2}}{d_M(z)}\right)^{kN} + \frac{\alpha^P}{d_M(z)} \right\} \end{aligned}$$

Since $p = \frac{2n}{k}$, this proves (B.7) for general N.

The proof of (B.7) for $N = 1$ is by induction after k; we start by proving the induction step. Let $n > 3$ be fixed, and let $k + 1 \le 2n$. Assume the bound (B.7) is satisfied for k. The idea of the proof of the bound (B.7) for for $k+1$ is to make use of the space between the supports of the functions χ and ϕ in the following way: Let $\eta \in C^\infty(\mathbb{R})$ be a monotone function such that $0 \le \eta \le 1$ and

$$\eta(t) = \begin{cases} 1 & t \le 1/3 \\ 0 & t \ge 2/3. \end{cases}$$

For some m to be determined later, define the following family of functions, $\chi^{(j)} \in C_0^\infty(\mathbb{R}^3), j = 1, 2, \ldots, m$:

$$\chi^{(j)}(x) = \eta\left(\frac{m}{\rho(\nu-1)}\left[|x| - \rho - \frac{\rho(\nu-1)(j-1)}{m}\right]\right) \tag{B.10}$$

This means, that

$$\chi^{(j)}(x) = \begin{cases} 1, & |x| \le \nu_1(j,m)\rho = \left(1 + \frac{(\nu-1)(j-2/3)}{m}\right)\rho \\ 0, & |x| \ge \nu_2(j,m)\rho = \left(1 + \frac{(\nu-1)(j-1/3)}{m}\right)\rho \end{cases} \tag{B.11}$$

with $\rho < \nu_1(j,m)\rho < \nu_2(j,m)\rho < \nu\rho$ and $\nu_2(j,m) < \nu_1(j+1,m)$. That is, $\chi^{(j+1)}\chi^{(j)} = \chi^{(j)}$ and $\chi^{(j)}\phi = 0$. Moreover, $\chi\chi^{(j)} = \chi$ for $j = 1, 2, \ldots, m$.

The idea is now to stick in $\chi^{(1)}$ after the χ in $\chi R(z,H)\phi$ and then commute it through:

$$\begin{aligned} \chi R(z,H)\phi &= \chi\chi^{(1)}R(z,H)\phi \\ &= \chi\chi^{(1)}R(z,H)\phi - \chi R(z,H)\chi^{(1)}\phi \\ &= -\chi[R(z,H),\chi^{(1)}]\phi = \chi R(z,H)[H,\chi^{(1)}]R(z,H)\phi. \end{aligned} \tag{B.12}$$

Now, had the commutator $[H, \chi^{(1)}]$ been local (as it is in the 'classical' case, with p^2 as kinetic energy), then we would have been able to stick in the $\chi^{(2)}$ after it: $[p^2,\chi^{(1)}] = [p^2,\chi^{(1)}]\chi^{(2)}$. We could then use the induction hypothesis on the factor $\chi^{(2)}R(z,H)\phi$ and gain the needed powers of β etc. from the factor $\chi R(z,H)[p^2,\chi^{(1)}]$. Now, in our case, the involved commutator will be that of $H_0 = \sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1}$ and $\chi^{(1)}$, which will not be local; we can therefore not stick in the $\chi^{(2)}$ after this commutator and iterate—at least not without paying for the non-locality.

To this end, we shall make use of the following expression for the square root:

Lemma B.3.

$$\sqrt{x} = -\frac{1}{\pi}\int_0^\infty \left(\frac{1}{x+t} - \frac{1}{t}\right)\sqrt{t}\,dt, \quad x \ge 0.$$

Proof. This follows from the calculation

$$\int_0^\infty \left(\frac{1}{x+t} - \frac{1}{t}\right)\sqrt{t}\,dt = -x\int_0^\infty \frac{\sqrt{t}\,dt}{t(x+t)}$$
$$= -\sqrt{x}\int_0^\infty \frac{2\,dy}{1+y^2} = -\pi\sqrt{x}$$

by the change of variables, $t = x/y^2$. □

Using the lemma, this means that

$$\begin{aligned}
&[H,\chi^{(1)}] = [\sqrt{\alpha^{-1}p^2+\alpha^{-2}},\chi^{(1)}] \\
&= -\frac{1}{\pi}\int_0^\infty [(\alpha^{-1}p^2+\alpha^{-2}+t)^{-1},\chi^{(1)}]\sqrt{t}\,dt \\
&= \frac{1}{\pi}\int_0^\infty (\alpha^{-1}p^2+\alpha^{-2}+t)^{-1}[\alpha^{-1}p^2,\chi^{(1)}](\alpha^{-1}p^2+\alpha^{-2}+t)^{-1}\sqrt{t}\,dt.
\end{aligned} \tag{B.13}$$

Note, that we have already repeatedly used the formula

$$[R(z,T),\phi] = -R(z,T)[T,\phi]R(z,T). \tag{B.14}$$

Using (B.12) and (B.13), we get that

$$\begin{aligned}
\chi R(z,H)\phi &= \chi R(z,H)[\sqrt{\alpha^{-1}p^2+\alpha^{-2}},\chi^{(1)}]R(z,H)\phi \\
&= \chi R(z,H)\frac{1}{\pi}\int_0^\infty \Big\{(\alpha^{-1}p^2+\alpha^{-2}+t)^{-1}[\alpha^{-1}p^2,\chi^{(1)}] \\
&\qquad \times (\alpha^{-1}p^2+\alpha^{-2}+t)^{-1}\sqrt{t}\Big\}\,dt\,R(z,H)\phi
\end{aligned}$$

Now, since $[\alpha^{-1}p^2,\chi^{(1)}] = [\alpha^{-1}p^2,\chi^{(1)}]\chi^{(2)}$, by commuting $\chi^{(2)}$ and $R_t = (\alpha^{-1}p^2+\alpha^{-2}+t)^{-1}$, we get that this equals

$$\begin{aligned}
&\left[\chi R(z,H)\frac{1}{\pi}\int_0^\infty R_tC_1R_t\sqrt{t}\,dt\right]\chi^{(2)}R(z,H)\phi \\
&\quad + \left[\chi R(z,H)\frac{1}{\pi}\int_0^\infty R_tC_1R_tC_2R_t\sqrt{t}\,dt\right]R(z,H)\phi
\end{aligned}$$

Here, $C_j = [\alpha^{-1}p^2,\chi^{(j)}]$. Of these two terms, we can use the induction hypothesis on the last factor of the first one, whereas we have to iterate the procedure above on the second; using that $C_2 = [\alpha^{-1}p^2,\chi^{(2)}] = [\alpha^{-1}p^2,\chi^{(2)}]\chi^{(3)} = C_2\chi^{(3)}$ we get, that

$$\begin{aligned}
\chi R(z,H)\phi = &\left[\chi R(z,H)\frac{1}{\pi}\int_0^\infty R_tC_1R_t\sqrt{t}\,dt\right]\chi^{(2)}R(z,H) \\
&+ \left[\chi R(z,H)\frac{1}{\pi}\int_0^\infty R_tC_1R_tC_2R_t\sqrt{t}\,dt\right]\chi^{(3)}R(z,H) \\
&+ \left[R(z,H)\frac{1}{\pi}\int_0^\infty R_tC_1R_tC_2R_tC_3R_t\sqrt{t}\,dt\right]R(z,H)
\end{aligned}$$

Continuing this way, we arrive at

$$\begin{aligned}
&\chi R(z,H)\phi \\
&\quad = \sum_{j=1}^{m-1} \left[\chi R(z,H) \frac{1}{\pi} \int_0^\infty R_t C_1 R_t \cdots R_t C_j R_t \sqrt{t}\, dt \right] \chi^{(j+1)} R(z,H)\phi \\
&\quad + \left[\chi R(z,H) \frac{1}{\pi} \int_0^\infty R_t C_1 R_t \cdots R_t C_m R_t \sqrt{t}\, dt \right] R(z,H)\phi \qquad \text{(B.15)}
\end{aligned}$$

To proceed, note that, since $p = -i\beta\nabla$, we have the operator equalities

$$\begin{aligned}
[p^2, \zeta] &= -i\beta\big(p \cdot \nabla\zeta + \nabla\zeta \cdot p\big) \\
&= -i\beta\big(2p \cdot \nabla\zeta + i\beta\Delta\zeta\big) \\
&= -i\beta\big(2\nabla\zeta \cdot p - i\beta\Delta\zeta\big) \qquad \text{(B.16)}
\end{aligned}$$

and so

$$\begin{aligned}
C_j R_t &= [\alpha^{-1}p^2, \chi^{(j)}](\alpha^{-1}p^2 + \alpha^{-2} + t)^{-1} \\
&= -i(\sqrt{\alpha}\beta)(2\,\nabla\chi^{(j)} \cdot (\sqrt{\alpha}p) - i\sqrt{\alpha}\beta\Delta\chi^{(j)})(\alpha p^2 + 1 + \alpha^2 t)^{-1}
\end{aligned}$$

By the spectral theorem,

$$\begin{aligned}
\|\sqrt{\alpha}p_l(\alpha p^2 + 1 + \alpha^2 t)^{-1}\| &\le \frac{1}{2\sqrt{1+\alpha^2 t}} \quad , \quad l = 1, 2, 3, \\
\|(\alpha p^2 + 1 + \alpha^2 t)^{-1}\| &\le \frac{1}{1+\alpha^2 t}
\end{aligned}$$

and so, by the definition of $\chi^{(j)}$, since all derivatives of η are supported in the interval $[1/3, 2/3]$, and since $\alpha \le \alpha_0$, $\beta \le \beta_0$, and $\rho \ge \rho_0$, we get that

$$\begin{aligned}
\|C_j R_t\| &\le (\sqrt{\alpha}\beta)\Big(\frac{\sum_{l=1}^3 \|\partial_l \chi^{(j)}\|_\infty}{\sqrt{1+\alpha^2 t}} + \frac{\sqrt{\alpha}\beta\, \|\Delta\chi^{(j)}\|_\infty}{1+\alpha^2 t} \Big) \\
&\le 3\sqrt{\alpha_0}\beta_0 \left(\frac{m}{\rho_0(\nu - 1)} \right) \|\eta'\|_\infty + 3\alpha_0\beta_0^2 \left(\frac{m}{\rho_0(\nu-1)} \right)^2 \|\eta''\|_\infty \\
&\quad + 3\alpha_0\beta_0^2 \frac{m}{\rho_0^2(\nu-1)} \|\eta'\|_\infty \\
&\equiv C(\alpha_0, \beta_0, \rho_0, \nu, \eta, m).
\end{aligned}$$

By the generalised Hölder inequality (3.2), and (3.1), this gives us, that

$$\begin{aligned}
&\left\| \left[\chi R(z,H) \frac{1}{\pi} \int_0^\infty R_t C_1 R_t \cdots R_t C_j R_t \sqrt{t}\, dt \right] \chi^{(j+1)} R(z,H)\phi \right\|_{\frac{2n}{k+1}} \\
&\leq \frac{1}{\pi} \int_0^\infty \| \chi R(z,H) R_t C_1 R_t \cdots R_t C_j R_t \|_{2n} \sqrt{t}\, dt \, \| \chi^{(j+1)} R(z,H)\phi \|_{\frac{2n}{k}} \\
&\leq \frac{1}{\pi} C(\alpha_0, \beta_0, \rho_0, \nu, \eta, m)^{j-1} \| \chi^{(j+1)} R(z,H)\phi \|_{\frac{2n}{k}} \\
&\qquad \times \int_0^\infty \| \chi R(z,H) R_t C_1 R_t \|_{2n} \sqrt{t}\, dt \qquad \text{(B.17)}
\end{aligned}$$

To bound the last factor in (B.17), we rewrite the operator $R(z,H)$ as follows:

$$\begin{aligned}
R(z,H) &= R(-\lambda, H_0)^{1/2} (H_0 + \lambda)^{1/2} R(z,H) (H_0 + \lambda)^{1/2} R(-\lambda, H_0)^{1/2} \\
&= R(-\lambda, H_0)^{1/2} S(\lambda, z) R(-\lambda, H_0)^{1/2} \qquad \text{(B.18)}
\end{aligned}$$

with

$$\begin{aligned}
S(\lambda, z) = (H_0 + \lambda)^{1/2} &R(-\lambda, H)^{1/2} (I + (\lambda + z) R(z,H)) \\
&\times R(-\lambda, H)^{1/2} (H_0 + \lambda)^{1/2} \qquad \text{(B.19)}
\end{aligned}$$

by the resolvent identity and since $R(-\lambda, H)^{1/2}$ and $R(z,H)$ commute. By the spectral theorem we have that

$$\| R(-\lambda, H_0)^{1/2} \| \leq \sup_{x \geq 0} (\sqrt{\alpha^{-1} x + \alpha^{-2}} - \alpha^{-1} + \lambda)^{-1/2} = \frac{1}{\sqrt{\lambda}}. \qquad \text{(B.20)}$$

Next, we recall that the potential V is assumed to satisfy (2) in Assumption B.1:

$$\big(|V|^{1/2} u, |V|^{1/2} u \big) \leq \varepsilon \big(H_0 u, u \big) + M(\beta, \alpha, \varepsilon) \big(u, u \big),$$

with $\varepsilon \in (0,1)$ and $M = M(\beta, \alpha, \varepsilon) \geq 1$, for all $u \in C_0^\infty(\mathbb{R}^3)$. This means, that as quadratic forms,

$$-\varepsilon H_0 - M \leq -|V| \leq V$$

and choosing $\lambda \geq M/\varepsilon$, we have, that

$$M + (1 - \varepsilon)\lambda \leq \lambda.$$

In this way,

$$\begin{aligned}
\big((H_0 + \lambda)^{1/2} \psi, (H_0 + \lambda)^{1/2} \psi \big) &= \big((H_0 + \lambda) \psi, \psi \big) \\
&= \frac{1}{1 - \varepsilon} \big((H_0 - \varepsilon H_0 - M + M + (1 - \varepsilon)\lambda) \psi, \psi \big) \\
&\leq \frac{1}{1 - \varepsilon} \big((H_0 + V + \lambda) \psi, \psi \big) = \frac{1}{1 - \varepsilon} \big((H + \lambda) \psi, \psi \big)
\end{aligned}$$

by the above, and so

$$\| (H_0 + \lambda)^{1/2} R(-\lambda, H)^{1/2} \| \leq \frac{1}{\sqrt{1 - \varepsilon}}$$

for $\lambda \geq M/\varepsilon$. Since

$$d_M(z) = \inf_{x\in[-M,\infty)} |z-x| \leq |z-(-M)| \leq |z| + M \leq |z| + \lambda.$$

we have that

$$\frac{\lambda + |z|}{d_M(z)} \geq 1.$$

This, the factorisation (B.19) and

$$\|R(z,H)\| \leq \frac{1}{d_M(z)}, \tag{B.21}$$

lead to the bound

$$\|S(\lambda,z)\| \leq \frac{2}{1-\varepsilon}\frac{\lambda+|z|}{d_M(z)}. \tag{B.22}$$

In this way, using (B.18) and that $0 \leq |\chi| \leq 1$, we get the estimate

$$\begin{aligned} \int_0^\infty \|\chi R(z,H)R_tC_1R_t\|_{2n}\sqrt{t}\,dt \leq{}& \frac{2}{1-\varepsilon}\frac{1}{\sqrt{\lambda}}\frac{\lambda+|z|}{d_M(z)} \\ &\times \int_0^\infty \|(H_0+\lambda)^{-1/2}R_tC_1R_t\|_{2n}\sqrt{t}\,dt. \end{aligned} \tag{B.23}$$

By the change of variable, $s = \alpha^2 t$, and with $q = \sqrt{\alpha}p = -i\sqrt{\alpha}\beta\nabla$, $\kappa = \alpha\lambda$, we have, by (B.16), that

$$\begin{aligned} &\int_0^\infty \|(H_0+\lambda)^{-1/2}R_tC_1R_t\|_{2n}\sqrt{t}\,dt \\ &= (\alpha^{-1}\beta)\int_0^\infty \|(\sqrt{\alpha^{-1}p^2+\alpha^{-2}}-\alpha^{-1}+\lambda)^{-1/2}(\alpha^{-1}p^2+\alpha^{-2}+t)^{-1} \\ &\qquad \times (p\cdot\nabla\chi^{(1)}+\nabla\chi^{(1)}\cdot p)(\alpha^{-1}p^2+\alpha^{-2}+t)^{-1}\|_{2n}\sqrt{t}\,dt \\ &= \beta\int_0^\infty \|(\sqrt{q^2+1}-1+\kappa)^{-1/2}(q^2+1+s)^{-1} \\ &\qquad \times (q\cdot\nabla\chi^{(1)}+\nabla\chi^{(1)}\cdot q)(q^2+1+s)^{-1}\|_{2n}\sqrt{s}\,ds \\ &= \beta\int_0^\infty \|(\sqrt{q^2+1}-1+\kappa)^{-1/2}(q^2+1+s)^{-1} \\ &\qquad \times (2q\cdot\nabla\chi^{(1)}+i\sqrt{\alpha}\beta\Delta\chi^{(1)})(q^2+1+s)^{-1}\|_{2n}\sqrt{s}\,ds \end{aligned} \tag{B.24}$$

Notice, that using (B.14) and (B.16), we get the formulae

$$
\begin{aligned}
&(q\cdot\nabla\chi^{(1)})(q^2+1+s)^{-1} = \sum_{l=1}^{3} q_l\,\partial_l\chi^{(1)}(q^2+1+s)^{-1}\\
&\quad = (q^2+1+s)^{-1}q\cdot\nabla\chi^{(1)}\\
&\qquad + 2(-i\sqrt{\alpha}\beta)\sum_{l=1}^{3} q_l(q^2+1+s)^{-1}\nabla(\partial_l\chi^{(1)})\cdot q(q^2+1+s)^{-1}\\
&\qquad - \alpha\beta^2(q^2+1+s)^{-1}q\cdot\nabla(\Delta\chi^{(1)})(q^2+1+s)^{-1}
\end{aligned}
\tag{B.25}
$$

and

$$
\begin{aligned}
&\Delta\chi^{(1)}(q^2+1+s)^{-1} = (q^2+1+s)^{-1}\Delta\chi^{(1)}\\
&\qquad + 2(-i\sqrt{\alpha}\beta)(q^2+1+s)^{-1}\nabla(\Delta\chi^{(1)})\cdot q(q^2+1+s)^{-1}\\
&\qquad - \alpha\beta^2(q^2+1+s)^{-1}\Delta(\Delta\chi^{(1)})(q^2+1+s)^{-1}.
\end{aligned}
\tag{B.26}
$$

We used that q_l and $(q^2+1+s)^{-1}$ commute for $l=1,2,3$. Using (B.25) and (B.26), (B.24) gives us, that

$$
\begin{aligned}
&\int_0^\infty \|(H_0+\lambda)^{-1/2}R_tC_1R_t\|_{2n}\sqrt{t}\,dt\\
&\leq \beta\Big\{\int_0^\infty \|(\sqrt{q^2+1}-1+\kappa)^{-1/2}(q^2+1+s)^{-1}\\
&\qquad\qquad \times 2(q^2+1+s)^{-1}q\cdot\nabla\chi^{(1)}\|_{2n}\sqrt{s}\,ds\\
&+ 4(\sqrt{\alpha}\beta)\sum_{l=1}^{3}\int_0^\infty \|(\sqrt{q^2+1}-1+\kappa)^{-1/2}(q^2+1+s)^{-1}\\
&\qquad \times q_l(q^2+1+s)^{-1}\nabla(\partial_l\chi^{(1)})\cdot q(q^2+1+s)^{-1}\|_{2n}\sqrt{s}\,ds\\
&+ 2(\alpha\beta^2)\int_0^\infty \|(\sqrt{q^2+1}-1+\kappa)^{-1/2}(q^2+1+s)^{-1}\\
&\qquad \times (q^2+1+s)^{-1}q\cdot\nabla(\Delta\chi^{(1)})(q^2+1+s)^{-1}\|_{2n}\sqrt{s}\,ds\\
&+ (\sqrt{\alpha}\beta)\int_0^\infty \|(\sqrt{q^2+1}-1+\kappa)^{-1/2}(q^2+1+s)^{-1}\\
&\qquad \times (q^2+1+s)^{-1}\Delta\chi^{(1)}\|_{2n}\sqrt{s}\,ds\\
&+ (\alpha\beta^2)\int_0^\infty \|(\sqrt{q^2+1}-1+\kappa)^{-1/2}(q^2+1+s)^{-1}\\
&\qquad \times 2(q^2+1+s)^{-1}\nabla(\Delta\chi^{(1)})\cdot q(q^2+1+s)^{-1}\|_{2n}\sqrt{s}\,ds\\
&+ (\alpha\sqrt{\alpha}\beta^3)\int_0^\infty \|(\sqrt{q^2+1}-1+\kappa)^{-1/2}(q^2+1+s)^{-1}\\
&\qquad \times (q^2+1+s)^{-1}\Delta(\Delta\chi^{(1)})(q^2+1+s)^{-1}\|_{2n}\sqrt{s}\,ds\Big\}.
\end{aligned}
\tag{B.27}
$$

Using the inequality $\|AB\|_{2n} \leq \|A\|_{2n}\|B\|$ (see (3.1)) on all, but the first and fourth term above, and the fact that by the spectral theorem, for $l = 1, 2, 3$, ($q_l = (-i\sqrt{\alpha}\beta)\,\partial_l$)

$$\begin{aligned} \|q_l(q^2+1+s)^{-1}\| &\leq \frac{1}{2\sqrt{1+s}} \leq \frac{1}{2} \\ \|(q^2+1+s)^{-1}\| &\leq \frac{1}{1+s} \leq 1, \end{aligned} \tag{B.28}$$

we are down to estimating the $2n$-Schatten class norm of operators of the form

$$(\sqrt{q^2+1}-1+\kappa)^{-1/2}(q^2+1+s)^{-2}\,\Phi$$

and

$$(\sqrt{q^2+1}-1+\kappa)^{-1/2}(q^2+1+s)^{-2}q\cdot\Psi$$

for various choices of functions Φ and Ψ $(\Delta\chi^{(1)}, \nabla(\Delta\chi^{(1)}), \ldots)$. To this end, we use the following lemma (see Reed and Simon [25, Thm. XI.20 p. 47]):

Lemma B.4. *Let $2 \leq r < \infty$ and suppose that $f, g \in L^r(\mathbb{R}^d)$. Then the operator $f(x)g(-i\nabla)$ is in $\mathfrak{S}_r$ (the r'th Schatten-class) and*

$$\|f(x)g(-i\nabla)\|_r \leq (2\pi)^{-d/r}\|f\|_{L^r}\|g\|_{L^r}.$$

Remark B.5. By scaling, this means, that

$$\|f(x)g(-i\beta\nabla)\|_r \leq (2\pi\beta)^{-d/r}\ \|f\|_{L^r}\|g\|_{L^r}.$$

That is, we need an estimate on

$$\|(\sqrt{q^2+1}-1+\kappa)^{-1/2}(q^2+1+s)^{-2}q_l\|_{L^{2n}}$$

and

$$\|(\sqrt{q^2+1}-1+\kappa)^{-1/2}(q^2+1+s)^{-2}\|_{L^{2n}}.$$

For this, note that, with $c = \sqrt{2}-1$,

$$\sqrt{y^2+1}-1 \geq \begin{cases} c\,y, & y \geq 1 \\ c\,y^2, & y \in [0,1] \end{cases} \tag{B.29}$$

and so, since $n > 3$ (and dropping κ), for $l = 1, 2, 3$:

$$\begin{aligned}
&\|(\sqrt{q^2+1} - 1 + \kappa)^{-1/2}(q^2+1+s)^{-2} q_l\|_{L^{2n}} \\
&\leq \frac{(4\pi)^{1/2n}}{\sqrt{c}} \Big\{ \int_0^1 \left| \frac{y}{\sqrt{y^2}(y^2+1+s)^2} \right|^{2n} y^2\, dy \\
&\qquad + \int_1^\infty \left| \frac{y}{\sqrt{y}(y^2+1+s)^2} \right|^{2n} y^2\, dy \Big\}^{1/2n} \\
&\leq \frac{(4\pi)^{1/2n}}{\sqrt{c}} (1+s)^{-\frac{7}{4}+\frac{3}{4n}} \Big\{ 1 + \int_1^\infty \frac{t^{n+2}\, dt}{(t^2+1)^{4n}} \Big\}^{1/2n} \\
&\leq \left(\frac{26}{25}\right)^{1/8} \frac{(4\pi)^{1/2n}}{\sqrt{c}} (1+s)^{-\frac{7}{4}+\frac{3}{4n}}.
\end{aligned}$$

Similarly (dropping $\sqrt{q^2+1} - 1$),

$$\begin{aligned}
&\|(\sqrt{q^2+1} - 1 + \kappa)^{-1/2}(q^2+1+s)^{-2}\|_{L^{2n}} \\
&\leq \left(4\pi \int_0^\infty \left| \frac{1}{\sqrt{\kappa}(y^2+1+s)^2} \right|^{2n} y^2\, dy \right)^{1/2n} \\
&= \frac{(4\pi)^{1/2n}}{\sqrt{\kappa}} (1+s)^{-2+\frac{3}{4n}} \left(\int_0^\infty (1+t^2)^{-4n} t^2\, dt \right)^{1/2n} \\
&\leq \left(\frac{30}{29}\right)^{1/8} \frac{(4\pi)^{1/2n}}{\sqrt{\kappa}} (1+s)^{-2+\frac{3}{4n}}.
\end{aligned}$$

In this way, since $n \geq 4$, by using Lemma B.4, we get

$$\begin{aligned}
&\int_0^\infty \|(\sqrt{q^2+1} - 1 + \kappa)^{-1/2}(q^2+1+s)^{-2} q \cdot \Psi\}\|_{2n} \sqrt{s}\, ds \\
&\leq (2\pi\sqrt{\alpha}\beta)^{-3/2n} \sum_{l=1}^3 \|\Psi_l\|_{L^{2n}} \left(\frac{26}{25}\right)^{1/8} \frac{(4\pi)^{1/2n}}{\sqrt{c}} \int_0^\infty (1+s)^{-\frac{7}{4}+\frac{3}{4n}} \sqrt{s}\, ds \\
&\leq C_1\, (\sqrt{\alpha}\beta)^{-3/2n} \sum_{l=1}^3 \|\Psi_l\|_{L^{2n}},
\end{aligned}$$

with $C_1 = (\frac{26}{25})^{1/8} \frac{17}{\sqrt{\sqrt{2}-1}}$. It is the convergence of the s-integral above that demands $n \geq 4$. Analogously, we have that

$$\begin{aligned}
&\int_0^\infty \|(\sqrt{q^2+1} - 1 + \kappa)^{-1/2}(q^2+1+s)^{-2}\, \Phi\}\|_{2n} \sqrt{s}\, ds \\
&\qquad \leq (2\pi\sqrt{\alpha}\beta)^{-3/2n} \|\Phi\|_{L^{2n}} \left(\frac{30}{29}\right)^{1/8} \frac{(4\pi)^{1/2n}}{\sqrt{\kappa}} \int_0^\infty (1+s)^{-2+\frac{3}{4n}} \sqrt{s}\, ds \\
&\qquad \leq \frac{C_2}{\sqrt{\kappa}}\, (\sqrt{\alpha}\beta)^{-3/2n} \|\Phi\|_{L^{2n}},
\end{aligned}$$

with $C_2 = \frac{21}{5}(\frac{30}{29})^{1/8}$. Looking at (B.27) we notice that all terms of the form right above (with Φ and not $q \cdot \Psi$) also contains a factor of $\sqrt{\alpha}$. Since $\lambda \geq M/\varepsilon \geq 1$, we have $\alpha/\kappa \leq 1$ ($\kappa = \alpha\lambda$).

In this way, taking into account (B.28), we finally get from (B.27) that

$$\begin{aligned}
&\int_0^\infty \|(H_0+\lambda)^{-1/2} R_t C_1 R_t\|_{2n} \sqrt{t}\, dt \\
&\leq \beta(\sqrt{\alpha}\beta)^{-\frac{3}{2n}} \Big\{ 2\, C_1 \Big(\sum_{l=1}^{3} \|\partial_l \chi^{(1)}\|_{L^{2n}} + (\sqrt{\alpha}\beta) \sum_{l,k=1}^{3} \|\partial_l \partial_k \chi^{(1)}\|_{L^{2n}} \\
&\qquad\qquad + (\alpha\beta^2) \sum_{l=1}^{3} \|\partial_l (\Delta\chi^{(1)})\|_{L^{2n}} \Big) \\
&\quad + C_2 \Big(\beta\, \|\Delta\chi^{(1)}\|_{L^{2n}} + \sum_{l=1}^{3} (\sqrt{\alpha}\beta^2) \|\partial_l(\Delta\chi^{(1)})\|_{L^{2n}} \\
&\qquad\qquad + (\alpha\beta^3) \|\Delta(\Delta\chi^{(1)})\|_{L^{2n}} \Big) \Big\} \qquad \text{(B.30)}
\end{aligned}$$

Recalling the definition (B.10) of $\chi^{(1)}$:

$$\chi^{(1)}(x) = \eta\left(\frac{m}{\rho(\nu-1)}\Big[|x| - \rho\Big]\right)$$

with

$$\eta(t) = \begin{cases} 1 & t \leq 1/3 \\ 0 & t \geq 2/3 \end{cases}$$

we see, that all derivatives of $\chi^{(1)}$ are supported in $\{|x| \geq \rho\}$, (see (B.11)) and so we get, that (with $\eta^{(j)}$ being the j'th derivative of η, $0 < |\gamma| \leq 4$, and C_γ an integer))

$$|\partial_x^\gamma \chi^{(1)}(x)| \leq \frac{C_\gamma}{\rho^{|\gamma|}} \left(\sum_{j=1}^{|\gamma|} \left(\frac{m}{\nu-1}\right)^j \left| \eta^{(j)}\left(\frac{m}{\rho(\nu-1)}\Big[|x|-\rho\Big]\right)\right| \right).$$

In this way,

$$\begin{aligned}
&\|\partial_x^\gamma \chi^{(1)}\|_{L^{2n}} \\
&\quad \leq \frac{C}{\rho^{|\gamma|}} \sum_{j=1}^{|\gamma|} \left(\frac{m}{\nu-1}\right)^j \left(4\pi \int_{y(t)\in[1/3,2/3]} |\eta^{(j)}(y(t))|^{2n}\, t^2\, dt\right)^{1/2n} \\
&\qquad\qquad \left(\quad y(t) = \frac{m}{\rho(\nu-1)}\Big(t-\rho\Big) \quad \right)
\end{aligned}$$

since $\operatorname{supp} \eta^{(j)} \subset [1/3, 2/3]$. Now, by the change of variable $y = y(t)$, and using that the integration then takes place over $y \in [1/3, 2/3]$, we get, since $\rho \geq \rho_0$, that (for $0 < |\gamma| \leq 4$)

$$\begin{aligned}
&\|\partial_x^\gamma \chi^{(1)}\|_{L^{2n}} \\
&\quad \leq C_\gamma\,(4\pi)^{1/2n}\,\rho^{\frac{3}{2n}-|\gamma|} \\
&\qquad \times \sum_{j=1}^{|\gamma|}\left(\frac{m}{\nu-1}\right)^j \left\{\left(\frac{\nu-1}{m}+1\right)^2\left(\frac{\nu-1}{m}\right)\right\}^{1/2n} \|\eta^{(j)}\|_{L^{2n}} \\
&\quad \leq \hat{C}\,\rho^{-1+\frac{3}{2n}}
\end{aligned} \tag{B.31}$$

with (since $n > 3$)

$$\begin{aligned}
\hat{C} &= C_4\,(1+\rho_0^{-1})^3(8\pi)^{1/8}\Big(1+\frac{m}{\nu-1}\Big)^4 \\
&\qquad \times \Big(2+\Big(\frac{\nu-1}{m}+\Big(\frac{\nu-1}{m}\Big)\Big)^{1/8}\Big)\Big(\sum_{j=1}^{4}\|\eta^{(j)}\|_{L^{2n}}\Big) \\
&= C(\rho_0, m, \nu, \eta) \quad (C_4 = \max_{|\gamma|\leq 4} C_\gamma).
\end{aligned} \tag{B.32}$$

Now, since $\alpha \leq \alpha_0$, $\beta \leq \beta_0$, (B.30) and (B.31) give us, that

$$\int_0^\infty \|(H_0+\lambda)^{-1/2}R_tC_1R_t\|_{2n}\sqrt{t}\,dt \leq \hat{\hat{C}}\,\frac{\beta}{\rho}\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^{\frac{3}{2n}} \tag{B.33}$$

with

$$\begin{aligned}
\hat{\hat{C}} &= (18\beta_0C_2+36C_1)(1+\alpha_0\beta_0^2)\,\hat{C}, \\
C_1 &= \left(\frac{26}{25}\right)^{1/8} \quad , \quad C_2 = \frac{21}{5}\left(\frac{30}{29}\right)^{1/8}
\end{aligned}$$

and $\hat{C}$ given by (B.32).

Combining this with (B.17) and (B.23), we arrive at the estimate

$$\begin{aligned}
&\left\|\left[\chi R(z,H)\frac{1}{\pi}\int_0^\infty R_tC_1R_t\cdots R_tC_jR_t\sqrt{t}\,dt\right]\chi^{(j+1)}R(z,H)\phi\right\|_{\frac{2n}{k+1}} \\
&\leq C\,\frac{1}{\sqrt{\lambda}}\,\frac{\lambda+|z|}{d_M(z)}\frac{\beta}{\rho}\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^{\frac{3}{2n}}\|\chi^{(j+1)}R(z,H)\phi\|_{\frac{2n}{k}}
\end{aligned} \tag{B.34}$$

Choosing $\lambda = |z| + M > M/\varepsilon$, (B.34) leads to the estimate

$$\begin{aligned}
&\left\|\left[\chi R(z,H)\frac{1}{\pi}\int_0^\infty R_tC_1R_t\cdots R_tC_jR_t\sqrt{t}\,dt\right]\chi^{(j+1)}R(z,H)\phi\right\|_{\frac{2n}{k+1}} \\
&\leq C\,\frac{(\,|z|+M\,)^{1/2}}{d_M(z)}\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^{\frac{3}{2n}}\left(\frac{\beta}{\rho}\right)\|\chi^{(j+1)}R(z,H)\phi\|_{\frac{2n}{k}}
\end{aligned} \tag{B.35}$$

We now turn to the last term in the decomposition (B.15):

$$\left[\chi R(z,H)\frac{1}{\pi}\int_0^\infty R_tC_1R_t\cdots R_tC_mR_t\sqrt{t}\,dt\right]R(z,H)\phi.$$

Rewriting $R(z,H)$ as in (B.18), using (B.16), and noting, with $q = \sqrt{\alpha}p = -i\sqrt{\alpha}\beta\nabla$, $\kappa = \alpha\lambda$ and

$$Q_l(y) = \left[(q^2+1+y)^{-1/2}\,q\right]\cdot\left[\nabla\chi^{(l)}(q^2+1+y)^{-1/2}\right] \tag{B.36}$$

that

$$\begin{aligned}R(-\lambda,H_0)^{1/2}&R_tC_1R_t\cdots R_tC_mR_tR(-\lambda,H_0)^{1/2}\\&=\alpha^3(-i\sqrt{\alpha}\beta)^m(\sqrt{q^2+1}-1+\kappa)^{-1/2}(q^2+1+\alpha^2t)^{-1/2}\\&\qquad\times\prod_{l=1}^m\left\{Q_l(\alpha^2t)+Q_l(\alpha^2t)^*\right\}\\&\qquad\times(q^2+1+\alpha^2t)^{-1/2}(\sqrt{q^2+1}-1+\kappa)^{-1/2}\end{aligned}$$

we get, upon making a change of variable, $s=\alpha^2t$, that

$$\begin{aligned}&\left[\chi R(z,H)\frac{1}{\pi}\int_0^\infty R_tC_1R_t\cdots R_tC_mR_t\sqrt{t}\,dt\right]R(z,H)\phi\\&=\chi R(-\lambda,H_0)^{1/2}S(\lambda,z)\frac{1}{\pi}\int_0^\infty(-i\sqrt{\alpha}\beta)^m(\sqrt{q^2+1}-1+\kappa)^{-1/2}\\&\times(q^2+1+s)^{-1/2}\Big(\prod_{l=1}^m\left\{Q_l(s)+Q_l(s)^*\right\}\Big)(q^2+1+s)^{-1/2}\\&\times(\sqrt{q^2+1}-1+\kappa)^{-1/2}\sqrt{s}\,ds\,S(\lambda,z)R(-\lambda,H_0)^{1/2}\phi\end{aligned}\tag{B.37}$$

By the spectral theorem,

$$\|(\sqrt{q^2+1}-1+\kappa)^{-1/2}(q^2+1+s)^{-1/2}\|\le\frac{1}{\sqrt{\kappa(1+s)}}=\frac{1}{\sqrt{\alpha\lambda(1+s)}} \tag{B.38}$$

and so by the generalised Hölder inequality (3.2), and (3.1), and the bound (B.22) on $S(\lambda,z)$, we get the estimate

$$\begin{aligned}&\left\|\left[\chi R(z,H)\frac{1}{\pi}\int_0^\infty R_tC_1R_t\cdots R_tC_mR_t\sqrt{t}\,dt\right]R(z,H)\phi\right\|_{\frac{2n}{k+1}}\\&\le(\sqrt{\alpha}\beta)^m\frac{1}{\alpha\lambda^2}\left(\frac{2(\lambda+|z|)}{(1-\varepsilon)\,d_M(z)}\right)^2\frac{1}{\pi}\int_0^\infty\prod_{l=1}^m\left(2\|Q_l(s)\|_{\frac{2nm}{k+1}}\right)\frac{ds}{\sqrt{1+s}}\end{aligned}$$

By the spectral theorem, for $j=1,2,3$ ($q_j=(-i\sqrt{\alpha}\beta)\partial_j$),

$$\|(q^2+1+s)^{-1/2}q_j\|\le 1,$$

and so, by Lemma B.4, we get that (see (B.36) for definition of Q_l)

$$
\begin{aligned}
\|Q_l(s)\|_{\frac{2nm}{k+1}} &\leq \sum_{j=1}^{3} \|(q^2+1+s)^{-1/2}\, q_j\| \\
&\quad \times (2\pi\sqrt{\alpha}\beta)^{-\frac{3(k+1)}{2nm}} \|(q^2+1+s)^{-1/2}\|_{L^{\frac{2nm}{k+1}}} \|\partial_j \chi^{(l)}\|_{L^{\frac{2nm}{k+1}}} \\
&\leq \sum_{j=1}^{3} (2\pi\sqrt{\alpha}\beta)^{-\frac{3(k+1)}{2nm}} \|(q^2+1+s)^{-1/2}\|_{L^{\frac{2nm}{k+1}}} \|\partial_j \chi^{(l)}\|_{L^{\frac{2nm}{k+1}}}
\end{aligned}
$$

Furthermore, since $k+1 \leq 2n$, for $m > 3$ we have

$$
\begin{aligned}
&\|(q^2+1+s)^{-1/2}\|_{L^{\frac{2nm}{k+1}}} \\
&= (1+s)^{-\frac{1}{2}+\frac{3(k+1)}{4nm}} \left\{ 4\pi \int_0^\infty \left| \frac{1}{\sqrt{t^2+1}} \right|^{\frac{2nm}{k+1}} t^2\, dt \right\}^{\frac{k+1}{2nm}} \\
&\leq (8\pi)^{\frac{k+1}{2nm}} (1+s)^{-\frac{1}{2}+\frac{3(k+1)}{4nm}}
\end{aligned}
$$

Finally, recall the definition of $\chi^{(l)}$:

$$
\chi^{(l)}(x) = \eta\left(\frac{m}{\rho(\nu-1)} \left[|x| - \rho - \frac{\rho(\nu-1)(l-1)}{m} \right] \right)
$$

and so, for $j = 1, 2, 3$,

$$
\frac{\partial \chi^{(l)}}{\partial x_j} = \left(\frac{m}{\rho(\nu-1)} \frac{x_j}{|x|} \right) \times \eta' \left(\frac{m}{\rho(\nu-1)} \left[|x| - \rho - \frac{\rho(\nu-1)(l-1)}{m} \right] \right).
$$

In this way,

$$
\begin{aligned}
\|\partial_j \chi^{(l)}\|_{L^{\frac{2nm}{k+1}}}^{\frac{2nm}{k+1}} &= \int_{\mathbb{R}^3} \left| \frac{\partial \chi^{(l)}}{\partial x_j}(x) \right|^{\frac{2nm}{k+1}} d^3x \\
&\leq \left(\frac{m}{\rho(\nu-1)} \right)^{\frac{2nm}{k+1}} 4\pi \int_{y(t)\in[1/3,2/3]} |\eta'(y(t))|^{\frac{2nm}{k+1}}\, t^2\, dt \\
\left(\quad y(t) \right. &= \left. \frac{m}{\rho(\nu-1)} \left(t - \rho - \frac{\rho(\nu-1)(l-1)}{m} \right) \quad \right)
\end{aligned}
$$

since $\operatorname{supp} \eta' \subset [1/3, 2/3]$. By the change of variable $y = y(t)$, and using that the integration then takes place over $y \in [1/3, 2/3]$, we get

(remember, that $l \leq m$)

$$\begin{aligned}
&\|\partial_j \chi^{(l)}\|_{L^{\frac{2nm}{k+1}}}^{\frac{2nm}{k+1}} \\
&\quad \leq \left(\frac{m}{\rho(\nu-1)}\right)^{\frac{2nm}{k+1}-1} \left(\rho + \frac{\rho(\nu-1)}{m} + \frac{\rho(\nu-1)(l-1)}{m}\right)^2 \\
&\qquad \times 4\pi \int_{1/3}^{2/3} |\eta'(y)|^{\frac{2nm}{k+1}}\, dy \\
&\quad \leq C\,\rho^{3-\frac{2nm}{k+1}}\ ,\ C = \left(\frac{m}{\nu-1}\right)^{\frac{2nm}{k+1}-1} \nu^2\, 4\pi\, \|\eta'\|_{L^{\frac{2nm}{k+1}}(\mathbb{R})}^{\frac{2nm}{k+1}}.
\end{aligned}$$

All of this gives the estimate

$$\|Q_l(s)\|_{\frac{2nm}{k+1}} \leq \frac{C}{\rho}\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^{\frac{3(k+1)}{2nm}} (1+s)^{-\frac{1}{2}+\frac{3(k+1)}{4nm}} \tag{B.39}$$

with

$$C = 3\left(\frac{m}{\nu-1}\right)^{1-\frac{k+1}{2nm}} \left(\frac{(2\nu)^2}{\pi}\right)^{\frac{k+1}{2nm}} \|\eta'\|_{L^{\frac{2nm}{k+1}}(\mathbb{R})}. \tag{B.40}$$

For $m > 4$, this leads to the bound

$$\begin{aligned}
&\left\|\left[\chi R(z,H)\frac{1}{\pi}\int_0^\infty R_t C_1 R_t \cdots R_t C_m R_t \sqrt{t}\, dt\right] R(z,H)\phi\right\|_{\frac{2n}{k+1}} \\
&\leq \tilde{C}\left(\frac{\sqrt{\alpha}\beta}{\rho}\right)^{m-\frac{3(k+1)}{2n}} \frac{1}{\alpha\lambda^2}\left(\frac{\lambda+|z|}{d_M(z)}\right)^2 \int_0^\infty (1+s)^{-\frac{m+1}{2}+\frac{3(k+1)}{4n}}\, ds \\
&\leq \tilde{C}\left(\frac{\sqrt{\alpha}\beta}{\rho}\right)^{m-\frac{3(k+1)}{2n}} \frac{1}{\alpha\lambda^2}\left(\frac{\lambda+|z|}{d_M(z)}\right)^2
\end{aligned}$$

with

$$\tilde{C} = 3\left(\frac{2}{1-\varepsilon}\right)^2 \frac{(6\,C)^m}{\pi}$$

where C is the constant from (B.40). As $k+1 \leq 2n$, we need $m > 4$ in order to ensure the convergence of the integral

$$\int_0^\infty (1+s)^{-\frac{m+1}{2}+\frac{3(k+1)}{4n}}\, ds.$$

Given $P \in \mathbb{N}$, we have, that

$$\begin{aligned}
&\left\| \left[\chi R(z,H) \frac{1}{\pi} \int_0^\infty R_t C_1 R_t \cdots R_t C_m R_t \sqrt{t}\, dt \right] R(z,H)\phi \right\|_{\frac{2n}{k+1}} \\
&\le \tilde{C}\, \frac{1}{d_M(z)} \left(\frac{\rho}{\sqrt{\alpha}\beta} \right)^{\frac{3(k+1)}{2n}} \left(\frac{\beta}{\rho} \right)^{k+1} \left\{ \left(\frac{\lambda + |z|}{\lambda} \right)^2 \frac{\alpha^P}{d_M(z)} \right\} \\
&\quad \times \left(\frac{\beta}{\rho} \right)^{m-(k+1)} \alpha^{\frac{m}{2}-1-P}.
\end{aligned}$$

Choosing now $m \ge \max\{2P+2, k+1, 5\}$, and remembering, that $\alpha \le \alpha_0, \beta \le \beta_0$ and $\rho \ge \rho_0$, we have (with $\lambda = |z| + M$), that

$$\begin{aligned}
&\left\| \left[\chi R(z,H) \frac{1}{\pi} \int_0^\infty R_t C_1 R_t \cdots R_t C_m R_t \sqrt{t}\, dt \right] R(z,H)\phi \right\|_{\frac{2n}{k+1}} \\
&\le \bar{C}\, \frac{1}{d_M(z)} \left(\frac{\rho}{\sqrt{\alpha}\beta} \right)^{\frac{3(k+1)}{2n}} \left(\frac{\beta}{\rho} \right)^{k+1} \left\{ \frac{\alpha^P}{d_M(z)} \right\} \qquad \text{(B.41)}
\end{aligned}$$

with

$$\begin{aligned}
\bar{C} = 4 &\left(\frac{2}{1-\varepsilon} \right)^2 \frac{6^m}{\pi} \left(\frac{\beta_0}{\rho_0} \right)^{m-(k+1)} \left(\sqrt{\alpha_0} \right)^{m-(2P+2)} \\
&\times \left(\frac{m}{\nu - 1} \right)^{m - \frac{k+1}{2n}} \left(\frac{(2\nu)^2}{\pi} \right)^{\frac{k+1}{2n}} \|\eta'\|^m_{L^{\frac{2nm}{k+1}}(\mathbb{R})}.
\end{aligned}$$

Notice, that the function η changes smoothly and monotonically from 1 to 0 on the interval $[1/3, 2/3]$ and so can be chosen such that $|\eta'| \le 6$. This means, that

$$\|\eta'\|^m_{L^{\frac{2nm}{k+1}}(\mathbb{R})} \le 6^m \left(\frac{1}{3} \right)^{\frac{k+1}{2n}}$$

and so we can, in (B.41), take

$$\begin{aligned}
\bar{C} = 4 &\left(\frac{2}{1-\varepsilon} \right)^2 \frac{36^m}{\pi} \left(\frac{\beta_0}{\rho_0} \right)^{m-(k+1)} \left(\sqrt{\alpha_0} \right)^{m-(2P+2)} \\
&\times \left(\frac{m}{\nu - 1} \right)^{m - \frac{k+1}{2n}} \left(\frac{(2\nu)^2}{3\pi} \right)^{\frac{k+1}{2n}}.
\end{aligned}$$

Recall the decomposition (B.15):

$$\begin{aligned}
&\chi R(z,H)\phi \\
&= \sum_{j=1}^{m-1} \left[\chi R(z,H) \frac{1}{\pi} \int_0^\infty R_t C_1 R_t \cdots R_t C_j R_t \sqrt{t}\, dt \right] \chi^{(j+1)} R(z,H)\phi \\
&+ \left[\chi R(z,H) \frac{1}{\pi} \int_0^\infty R_t C_1 R_t \cdots R_t C_m R_t \sqrt{t}\, dt \right] R(z,H)\phi.
\end{aligned}$$

Let

$$X = \frac{(\,|z| + M\,)^{1/2}}{d_M(z)} \quad , \quad Y = \frac{\alpha^P}{(\,|z| + M\,)^{1/2}} \le \alpha_0^P$$

then,

$$XY = \frac{\alpha^P}{d_M(z)}$$

and so, using the induction hypothesis, the bound (B.35) reads:

$$\begin{aligned}
&\left\| \left[\chi R(z,H) \frac{1}{\pi} \int_0^\infty R_t C_1 R_t \cdots R_t C_j R_t \sqrt{t}\, dt \right] \chi^{(j+1)} R(z,H)\phi \right\|_{\frac{2n}{k+1}} \\
&\le C\, \frac{(\,|z| + M\,)^{1/2}}{d_M(z)} \left(\frac{\rho}{(\sqrt{\alpha}\beta} \right)^{\frac{3}{2n}} \left(\frac{\beta}{\rho} \right) \|\chi^{(j+1)} R(z,H)\phi\|_{\frac{2n}{k}} \\
&\le C\, \frac{1}{d_M(z)} \left(\frac{\rho}{\sqrt{\alpha}\beta} \right)^{\frac{3(k+1)}{2n}} \left(\frac{\beta}{\rho} \right)^{k+1} X \left\{ X^k + XY \right\}.
\end{aligned}$$

Combining this with (B.41) gives the estimate

$$\begin{aligned}
&\|\chi R(z,H)\phi\|_{\frac{2n}{k+1}} \\
&\quad \le C\, \frac{1}{d_M(z)} \left(\frac{\rho}{\sqrt{\alpha}\beta} \right)^{\frac{3(k+1)}{2n}} \left(\frac{\beta}{\rho} \right)^{k+1} \left\{ X^{k+1} + X^2 Y + XY \right\} \qquad \text{(B.42)}
\end{aligned}$$

We get, that

$$\begin{aligned}
X^{k+1} + X^2 Y + XY &\le X^{k+1}(1+Y) + XY(1+X) \\
&= X^{k+1} + XY(1 + X + X^k) \le X^{k+1} + XY(1+X)^k \\
&\le X^{k+1} + XY\big(C_k(1+X^k)\big) \le \tilde{C}\big(X^{k+1} + XY\big).
\end{aligned}$$

with $C_k = 2^{k-1}$, since

$$(1+x)^{\frac{p}{q}} \le \max\{2^{\frac{p}{q}-1}, 1\}(1 + x^{\frac{p}{q}}) \qquad \forall p, q \in \mathbb{N} \quad , \quad \forall x \ge 0. \quad \text{(B.43)}$$

To prove this, look at the ratio of the expressions on the right- and left hand side, and differentiate. All this finally leads us to the estimate

$$\begin{aligned}
&\|\chi R(z,H)\phi\|_{\frac{2n}{k+1}} \\
&\quad \le C\, \frac{1}{d_M(z)} \left(\frac{\rho}{\sqrt{\alpha}\beta} \right)^{\frac{3(k+1)}{2n}} \left(\frac{\beta}{\rho} \right)^{k+1} \left\{ X^{k+1} + XY \right\}. \qquad \text{(B.44)}
\end{aligned}$$

Inserting the values of X and Y in (B.44), this gives exactly (B.7) for $k+1$ (and $N = 1$). This proves the the induction step.

The proof of the induction basis is easy now. We still decompose as in (B.15). The terms in the sum are bounded like in (B.17), just by using (3.1) and not the generalised Hölder inequality (3.2):

$$\begin{aligned}
&\left\| \left[\chi R(z,H) \frac{1}{\pi} \int_0^\infty R_t C_1 R_t \cdots R_t C_j R_t \sqrt{t}\, dt \right] \chi^{(j+1)} R(z,H)\phi \right\|_{2n} \\
&\leq C \, \|\chi^{(j+1)} R(z,H)\phi\| \\
&\qquad \times \int_0^\infty \|\chi R(z,H) R_t C_1 R_t\|_{2n} \sqrt{t}\, dt.
\end{aligned}$$

Bounding the first factor simply by $(d_M(z))^{-1}$ (see (B.21)) and the second using (B.23) and (B.33), using as before $\lambda = |z| + M/\varepsilon$, this is bounded by

$$C \frac{1}{d_M(z)} \left(\frac{\rho}{\sqrt{\alpha}\beta} \right)^{\frac{3}{2n}} \left(\frac{\beta}{\rho} \right)^1 \left(\frac{(\,|z| + M\,)^{1/2}}{d_M(z)} \right)^1 .$$

The last term in (B.15) is also treated as before — everything goes through, right till (B.41), just using $k = 0$ (so that $k + 1 = 1$). This gives a bound of

$$C \frac{1}{d_M(z)} \left(\frac{\rho}{\sqrt{\alpha}\beta} \right)^{\frac{3}{2n}} \left(\frac{\beta}{\rho} \right)^1 \left\{ \frac{\alpha^P}{d_M(z)} \right\}.$$

This proves (B.7) for $k = 1$, and therefore for general k by induction.

To prove (B.9), do as for (B.7) and note, that using the operator norm inequality $\|AB\| \leq \|A\| \, \|B\|$ instead of the generalised Hölder inequality (3.2), and (3.1), the bound (B.17) combined with (B.23) gives

$$\begin{aligned}
&\left\| \left[\chi R(z,H) \frac{1}{\pi} \int_0^\infty R_t C_1 R_t \cdots R_t C_j R_t \sqrt{t}\, dt \right] \chi^{(j+1)} R(z,H)\phi \right\| \\
&\qquad \leq C \, \|\chi^{(j+1)} R(z,H)\phi\| \int_0^\infty \|\chi R(z,H) R_t C_1 R_t\| \sqrt{t}\, dt \\
&\qquad \leq C \, \|\chi^{(j+1)} R(z,H)\phi\| \int_0^\infty \|\chi R(z,H) R_t C_1 R_t\| \sqrt{t}\, dt \\
&\qquad \leq C \, \|\chi^{(j+1)} R(z,H)\phi\| \frac{1}{\sqrt{\lambda}} \frac{\lambda + |z|}{d_M(z)} \\
&\qquad\qquad \times \int_0^\infty \|(H_0 + \lambda)^{-1/2} R_t C_1 R_t\| \sqrt{t}\, dt
\end{aligned}$$

Remains to bound the last factor above, similar to the bound (B.33), but in norm instead of the $2n$-Schatten-class norm (and then use the induction hypothesis). To do this, we only need to estimate in norm operators of the form

$$(\sqrt{q^2+1} - 1 + \kappa)^{-1/2} (q^2 + 1 + s)^{-2} \, \Phi$$

and

$$(\sqrt{q^2+1} - 1 + \kappa)^{-1/2} (q^2 + 1 + s)^{-2} q \cdot \Psi.$$

Doing as when estimating the Schatten-class norm of these (using (B.29) and dropping κ and $\sqrt{q^2+1}-1$ respectively) and again noting, that the resulting factor of $\kappa^{-\frac{1}{2}}$ cancels, we get a bound that reads

$$\int_0^\infty \|(H_0+\lambda)^{-1/2}R_t C_1 R_t\| \sqrt{t}\, dt \leq C\, \frac{\beta}{\rho}.$$

Basically, the difference is the lack of the factor $(\frac{\rho}{\sqrt{\alpha\beta}})^{\frac{3}{2n}}$ that occurs when dealing with Schatten-class norms and not operator norms; it stems from the use of the Lemma B.4. Same thing for the bound (B.41); here we need to notice (which we will also need for later use), that for (see (B.36))

$$Q_l(y) = \left[(q^2+1+y)^{-1/2}\, q\right]\cdot\left[\nabla\chi^{(l)}(q^2+1+y)^{-1/2}\right]$$

we have the bound

$$\begin{aligned}\|Q_l(y)\| &\leq \sum_{l=1}^{3} \|(q^2+1+y)^{-1/2}q_l\|\, \|\partial_l\chi^{(l)}\|\, \|(q^2+1+y)^{-1/2}\| \\ &\leq \sum_{l=1}^{3} \|\partial_l\chi^{(l)}\| \frac{1}{\sqrt{1+y}} \leq \frac{C}{\rho}\frac{1}{\sqrt{1+y}}. \end{aligned} \tag{B.45}$$

Again, the only difference from the Schatten-class case is the lack of (a power of) the factor $\left(\frac{\rho}{\sqrt{\alpha\beta}}\right)^{\frac{3}{2n}}$, see (B.39), and additionally, a positive factor of $1+y$, stemming from the same effect. The lack of the last only makes the convergence of the involved integrals (in y) better; in particular, (B.9) holds for all $N \geq 1$. □

Note the following:

Lemma B.6. *Assume the function X satisfies (B.4):*

$$\|Xu\|^2 \leq \varepsilon\big(H_0 u, u\big) + M(\beta,\alpha,\varepsilon)\|u\|^2 \quad \forall u \in C_0^\infty(\mathbb{R}^3)$$

for some $\varepsilon \in]0,1[$, $M(\beta,\alpha,\varepsilon) \geq 1$. Then

$$\|XR(z,H)\| \leq C\, \frac{(\,|z| + M\,)^{1/2}}{d_M(z)}. \tag{B.46}$$

Proof. For $\lambda \geq M/\varepsilon$, with $S(\lambda, z)$ as in (B.19).

$$\|XR(z,H)\| \leq \|XR(-\lambda,H_0)^{1/2}\|\, \|S(\lambda,z)\|\, \|R(-\lambda,H_0)^{1/2}\|.$$

Recall (B.22):

$$\|S(\lambda,z)\| \leq \frac{2}{1-\varepsilon}\frac{\lambda+|z|}{d_M(z)}$$

and that by the spectral theorem

$$\|R(-\lambda,H_0)^{1/2}\| \leq \frac{1}{\sqrt{\lambda}}.$$

Rests to bound the factor $\|XR(-\lambda, H_0)^{1/2}\|$. To this end, note, that by assumption,

$$\begin{aligned}\big(Xu, Xu\big) &\le \varepsilon\big(H_0u, u\big) + M\,\|u\|^2 = \varepsilon\Big\{\big(H_0u, u\big) + \frac{M}{\varepsilon}\|u\|^2\Big\} \\ &\le \varepsilon\Big\{\big(H_0u, u\big) + \lambda\|u\|^2\Big\} = \varepsilon\big((H_0+\lambda)^{1/2}u, (H_0+\lambda)^{1/2}u\big)\end{aligned}$$

and so

$$\|XR(-\lambda, H_0)^{1/2}\| \le \sqrt{\varepsilon}.$$

This proves the lemma, with $C = \frac{4}{1-\varepsilon}$ for $\lambda = |z| + M/\varepsilon$. □

The same idea permits us to prove a result related to Lemma B.2:

Lemma B.7. *Let the function X satisfy*

$$\|Xu\|^2 \le \varepsilon\big(H_0u, u\big) + M(\beta, \alpha, \varepsilon)\|u\|^2 \quad \forall u \in C_0^\infty(\mathbb{R}^3)$$

for some $\varepsilon \in]0,1[$, $M(\beta,\alpha,\varepsilon) \ge 1$ and let $K > 3$. Then, for any functions χ and ϕ satisfying (B.6),

$$\begin{aligned}\|X\chi\, R(z,H)\,\phi\|_1 \le C\,\frac{(\,|z| + M\,)^{1/2}}{d_M(z)}\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3\left(\frac{\beta}{\rho}\right)^{2K} \\ \times\left\{\left(\frac{(\,|z|+M\,)^{1/2}}{d_M(z)}\right)^{2K} + \frac{\alpha^P}{d_M(z)}\right\}\end{aligned} \tag{B.47}$$

Proof. All we need to notice is that the difference from the proof of Lemma B.2 is that the decomposition (B.18) will give rise to a first factor of $X\chi\, R(-\lambda, H_0)^{1/2}$ and not merely $\chi\, R(-\lambda, H_0)^{1/2}$. Since

$$\begin{aligned}\|X\chi\, R(-\lambda, H_0)^{1/2}\| &\le \sqrt{\varepsilon} \\ \|\chi\, R(-\lambda, H_0)^{1/2}\| &\le \frac{1}{\sqrt{\lambda}}\end{aligned}$$

(see proof of Lemma B.6) this gives, with the usual choice of $\lambda = |z| + M/\varepsilon$, rise to a factor of $(\,|z| + M\,)^{1/2}$ compared to the estimate (B.8) of Lemma B.2. This gives exactly the bound (B.47). □

The result (B.8) of Lemma B.2 generalises to any (positive integer) power of the resolvent by induction:

Lemma B.8. *Let χ and ϕ satisfy (B.6). Then for all $k \ge 1$, $K > 3$ and $P \ge 1$:*

$$\begin{aligned}\|\chi\, R(z,H)^k\,\phi\|_1 \le C\,\frac{1}{d_M(z)^k}\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3\left(\frac{\beta}{\rho}\right)^{2K} \\ \times\left\{\left(\frac{(\,|z|+M\,)^{1/2}}{d_M(z)}\right)^{2K} + \frac{\alpha^P}{d_M(z)}\right\}\end{aligned} \tag{B.48}$$

Proof. The proof is by induction after k; the induction basis, $k = 1$, is (B.8) of Lemma B.2.

Assume that the estimate (B.48) holds for some k. Choose a function χ_1 with $\operatorname{supp}\chi_1 \subset B(\frac{(1+2\nu)\rho}{3})$ such that $|\chi_1| \le 1$ and

$$\chi_1(x) = 1, \qquad |x| \le \frac{(2+\nu)}{3}\rho$$

and let $\phi_1 = 1 - \chi_1$. Since $\nu > 1$, we have that

$$\rho < \left(\frac{2+\nu}{3}\right)\rho < \left(\frac{1+2\nu}{3}\right)\rho < \nu\rho. \tag{B.49}$$

This means that the pairs of functions, χ_1, ϕ and χ, ϕ_1 satisfy the condition (B.6) of Lemma B.2; for the pair χ_1, ϕ, the values of (ρ, ν) are $(\frac{1+2\nu}{3}\rho, \frac{3\nu}{1+2\nu})$, for the pair χ, ϕ_1 they are $(\rho, \frac{2+\nu}{3})$. This gives the same dependence on ρ (and on ρ_0, due to (B.49)), but the constant, which depends on ν, will be different. This means, by (3.1), that

$$\begin{aligned} \|\chi R(z,H)^{k+1}\phi\|_1 &= \|\chi R(z,H)^k(\chi_1 + \phi_1)R(z,H)\phi\|_1 \\ &\le \|\chi R(z,H)^k\|\,\|\chi_1 R(z,H)\phi\|_1 \\ &\quad + \|\chi R(z,H)^k\phi_1\|_1\,\|R(z,H)\phi\|. \end{aligned} \tag{B.50}$$

Using that (see (B.21))

$$\|R(z,H)^k\| \le \frac{1}{d_M(z)^k} \quad , \quad \forall k \in \mathbb{N}, \tag{B.51}$$

the first term in (B.50) satisfies the estimate (B.48) for $k+1$ due to (B.8) of Lemma B.2, and so does the second one, due to the induction hypothesis. The lemma now follows by induction. ☐

This will allow us to prove the following:

Lemma B.9. *Let χ satisfy (B.6): $\operatorname{supp}\chi \subset B(\rho)$ and $|\chi| \le 1$, for $\rho \ge \rho_0$, and assume $0 < \alpha \le \alpha_0$ and $0 < \beta \le \beta_0$. Let $k, n \in \mathbb{N}$ be such that $n > 3, k \le 2n$. Then, with $p = \frac{2n}{k}$, we have the estimate*

$$\|\chi R(\pm iM, H)^k\|_p \le C\,M^{-k}\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^{\frac{3}{p}}\left(1 + (\alpha M)^{\frac{3}{p}}\right) \tag{B.52}$$

Proof. By induction after k. Let $k = 1$. Then

$$\|\chi R(\pm iM, H)\|_{2n} \le \|\chi R(-\lambda, H_0)^{1/2}\|_{2n}\,\|S(\lambda, \pm iM)\|\,\|R(-\lambda, H_0)^{1/2}\|$$

with S as in (B.19) and $\lambda \ge M/\varepsilon$. Now, by (B.22) and since $d_M(\pm iM) = M$, we have that

$$\|S(\lambda, \pm iM)\| \le \frac{2}{1-\varepsilon}\frac{\lambda + |\pm iM|}{d_M(\pm iM)} = \frac{2+4\varepsilon}{\varepsilon - \varepsilon^2}$$

for $\lambda = |\pm iM| + M/\varepsilon$, and by the spectral theorem (see (B.20))

$$\|R(-\lambda, H_0)^{1/2}\| \leq \frac{1}{\sqrt{\lambda}} = \frac{\sqrt{\varepsilon}}{\sqrt{1+\varepsilon}} \frac{1}{\sqrt{M}}.$$

Finally, by Lemma B.4,

$$\|\chi R(-\lambda, H_0)^{1/2}\|_{2n} \leq (2\pi\beta)^{-\frac{3}{2n}} \|\chi\|_{L^{2n}} \|g\|_{L^{2n}}$$

with

$$g(x) = \left(\sqrt{\alpha^{-1}x^2 + \alpha^{-2}} - \alpha^{-1} + \lambda\right)^{-1/2}.$$

Now, by the change of variables, $y = \sqrt{\alpha}\, t$,

$$\begin{aligned}\|g\|_{L^{2n}}^{2n} &= 4\pi \int_0^\infty \frac{t^2\, dt}{(\sqrt{\alpha^{-1}t^2 + \alpha^{-2}} - \alpha^{-1} + \lambda)^n} \\ &= \alpha^{n-\frac{3}{2}}\, 4\pi \int_0^\infty \frac{y^2\, dy}{(\sqrt{y^2+1} - 1 + \alpha\lambda)^n}\end{aligned}$$

To find the behaviour of the integral

$$\int_0^\infty \frac{y^2\, dy}{(\sqrt{y^2+1} - 1 + \kappa)^n}$$

as a function of κ, we again use, that

$$\sqrt{y^2+1} - 1 \geq \begin{cases} c\, y, & y \geq 1 \\ c\, y^2, & y \in [0,1] \end{cases}$$

with $c = \sqrt{2} - 1$. This means, that

$$\begin{aligned}\int_0^\infty \frac{y^2\, dy}{(\sqrt{y^2+1} - 1 + \kappa)^n} \leq\; & c^{-3/2} \kappa^{\frac{3}{2}-n} \int_0^{\sqrt{\frac{c}{\kappa}}} \frac{t^2\, dt}{(t^2+1)^n} \\ & + c^{-3} \kappa^{3-n} \int_{c/\kappa}^\infty \frac{t^2\, dt}{(t+1)^n}\end{aligned}$$

(by the changes of variables, $t = \sqrt{\frac{c}{\kappa}}\, y$, $t = \frac{c}{\kappa}\, y$, respectively).

Now,

$$\int_0^{\sqrt{\frac{c}{\kappa}}} \frac{t^2\, dt}{(t^2+1)^n} \leq \int_0^{\sqrt{\frac{c}{\kappa}}} t^2\, dt = \frac{1}{3} c^{3/2} \kappa^{-\frac{3}{2}}$$

and

$$\int_{c/\kappa}^\infty \frac{t^2\, dt}{(t+1)^n} \leq \int_0^\infty \frac{t^2\, dt}{(t+1)^n} \leq 2$$

since $n > 3$, and therefore

$$\int_0^\infty \frac{y^2\, dy}{(\sqrt{y^2+1} - 1 + \kappa)^n} \leq \kappa^{-n} \Big(\frac{1}{3} + \frac{2}{5\sqrt{2} - 7} \kappa^3 \Big).$$

Still with $\lambda = |\pm iM| + M/\varepsilon$, and using that (see (B.43))

$$(1+x)^r \leq \max\{2^{r-1}, 1\}(1 + r^r) \quad \forall x \geq 0 \quad , \quad \forall r \in \mathbb{Q}_+,$$

we get, that ($\kappa = \alpha\lambda$)

$$\|g\|_{L^{2n}} \le C\,\alpha^{-\frac{3}{4n}} M^{-\frac{1}{2}} \Big(1 + (\alpha M)^{\frac{3}{2n}}\Big).$$

Since $\operatorname{supp}\chi \subset B(\rho)$, $|\chi| \le 1$, we have, that $\|\chi\|_{L^{2n}} \le (\frac{4\pi}{3})^{1/2n} \rho^{\frac{3}{2n}}$, and so we get the estimate

$$\|\chi R(\pm iM, H)\|_{2n} \le C\, M^{-1} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^{\frac{3}{2n}} \Big(1 + (\alpha M)^{\frac{3}{2n}}\Big).$$

This proves the induction basis.

Assume now, that the estimate (B.52) holds for some k. Let χ_1 be a function with $\operatorname{supp}\chi_1 \subset B(3\rho)$ such that $\chi_1(x) = 1$ for $|x| \le 2\rho$ and $|\chi_1| \le 1$, and let $\phi = 1 - \chi_1$. Then the pair of functions χ, ϕ satisfies the conditions of Lemma B.2, and χ and χ_1 those of this lemma (the latter with 3ρ, instead of ρ), and so, by the generalised Hölder inequality (3.2), and (3.1),

$$\begin{aligned}\|\chi R(\pm iM, H)^{k+1}\|_{\frac{2n}{k+1}} &= \|\chi R(\pm iM, H)(\phi + \chi_1) R(\pm iM, H)^k\|_{\frac{2n}{k+1}} \\ &\le \|\chi R(\pm iM, H)\phi\|_{\frac{2n}{k+1}} \|R(\pm iM, H)^k\| \\ &\quad + \|\chi R(\pm iM, H)\|_{2n} \|\chi_1 R(\pm iM, H)^k\|_{\frac{2n}{k}}.\end{aligned}$$

Now, by (B.51) and (B.7) in Lemma B.2 (for $k+1$, and with $N = 1$) the first term above is bounded by

$$\begin{aligned}&\frac{C}{d_M(\pm iM)} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^{\frac{3(k+1)}{2n}} \left(\frac{\beta}{\rho}\right)^{k+1} \\ &\qquad \times \left\{ \left(\frac{(2M)^{1/2}}{d_M(\pm iM)}\right)^{k+1} + \frac{\alpha^P}{d_M(\pm iM)} \right\} \left\{ \frac{1}{d_M(\pm iM)^k} \right\} \\ &\le C\, M^{-(k+1)} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^{\frac{3(k+1)}{2n}},\end{aligned}$$

using, that $\alpha \le \alpha_0$, $\beta \le \beta_0$, $\rho \ge \rho_0$ and $M \ge 1$.

By the induction basis and the induction hypothesis (and using again (B.43)), the second term is bounded by

$$\begin{aligned}&\left\{ \frac{C}{M} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^{\frac{3}{2n}} \Big(1 + (\alpha M)^{\frac{3}{2n}}\Big) \right\} \left\{ \frac{C}{M^k} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^{\frac{3k}{2n}} \Big(1 + (\alpha M)^{\frac{3k}{2n}}\Big) \right\} \\ &\le C\, M^{-(k+1)} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^{\frac{3(k+1)}{2n}} \Big(1 + (\alpha M)^{\frac{3(k+1)}{2n}}\Big)\end{aligned}$$

In this way,

$$\|\chi R(\pm iM, H)^{k+1}\|_{\frac{2n}{k+1}} \le C\, M^{-(k+1)} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^{\frac{3(k+1)}{2n}} \Big(1 + (\alpha M)^{\frac{3(k+1)}{2n}}\Big)$$

which is (B.52) for $k+1$; the lemma now follows by induction. $\square$

Using the above lemma, we can prove the first result on local Riesz means of H:

Lemma B.10. *Let χ be as before:* $\operatorname{supp}\chi \subset B(\rho)$, $|\chi| \le 1$, $\rho \ge \rho_0$. *Let $g = g(\lambda)$ be a function such that $g(\lambda) = 0$, $\lambda \ge \lambda_0$ and $|g(\lambda)| \le C_{g,s}|\lambda|^s$ for some (fixed) $s \ge 0$. Then*

$$\|\chi g(H)\|_1 \le C\, M^s \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \big(1 + (\alpha M)^3\big). \tag{B.53}$$

Remark B.11. We are mainly interested in the case $s = 1$, namely for (a smoothed out version of) the function $|x|_- = \max\{0, -x\}$.

Proof. From Lemma B.9 with $k = 2n > 6$ we get, using (3.1) that

$$\begin{aligned}\|\chi g(H)\|_1 &\le \|\chi R(iM,H)^k\|_1 \|(H - iM)^k g(H)\| \\ &\le C\, M^{-k} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \big(1 + (\alpha M)^3\big)\, \|(H - iM)^k g(H)\|.\end{aligned}$$

Now, by the spectral theorem,

$$\|(H - iM)^k g(H)\| \le \|f\|_\infty$$

with

$$f(\lambda) = (\lambda - iM)^k g(\lambda)\ , \qquad \lambda \in [-M, \lambda_0].$$

Using that $|g(\lambda)| \le C_{g,s}|\lambda|^s$, and that $M \ge 1$, we get, that $\|f\|_\infty \le C\, M^{s+k}$, with $C = C_{g,s}\sqrt{2 + \lambda_0^2}\,(1 + \lambda_0)^s$. This proves the lemma. $\square$

We will eventually need the following lemma, which relates to Lemma B.7 and Lemma B.9.

Lemma B.12. *Let, as before,* $\operatorname{supp}\chi \subset B(\rho)$, $|\chi| \le 1$, *with* $\rho \ge \rho_0$, *and let the function X satisfy*

$$\|Xu\|^2 \le \varepsilon\big(H_0 u, u\big) + M(\beta, \alpha, \varepsilon)\|u\|^2 \quad \forall u \in C_0^\infty(\mathbb{R}^3)$$

for some $\varepsilon \in]0,1[$ and $M = M(\beta, \alpha, \varepsilon) \ge 1$. Then for any $k > 6$

$$\|X\chi R(\pm iM, H)^{k+1}\|_1 \le C\, M^{-k-\frac{1}{2}} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \big(1 + (\alpha M)^3\big). \tag{B.54}$$

Proof. Let χ_1, $\operatorname{supp}\chi_1 \subset B(3\rho)$, $|\chi_1| \le 1$, $\chi_1(x) = 1$ for $|x| \le 2\rho$, be the function from the proof of the induction step in the proof of Lemma B.9, and let $\phi = 1 - \chi_1$. Then

$$\begin{aligned}\|X\chi R(\pm iM, H)^{k+1}\|_1 \le{}& \|X\chi R(\pm iM, H)\phi\|_1 \|R(\pm iM, H)^k\| \\ &+ \|X\chi R(\pm iM, H)\|\, \|\chi_1 R(\pm iM, H)^k\|_1.\end{aligned}$$

By Lemma B.6 and Lemma B.9 (with $2n = k > 6$), the second term is bounded by

$$C\, \frac{(2M)^{1/2}}{d_M(\pm iM)} \times M^{-k} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \big(1 + (\alpha M)^3\big)$$

whereas by Lemma B.7 and (B.51), the first term is (for $K > 3$) bounded by

$$C \frac{(2M)^{1/2}}{d_M(\pm iM)} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \left(\frac{\beta}{\rho}\right)^{2K} \\ \times \left\{ \left(\frac{(2M)^{1/2}}{d_M(\pm iM)}\right)^{2K} + \frac{\alpha^P}{d_M(\pm iM)} \right\} M^{-k}.$$

Using, that $\alpha \leq \alpha_0$, $\beta \leq \beta_0$, $\rho \geq \rho_0$ and $M \geq 1$, this provides, for both terms, the bound (B.54). $\square$

Until now, we have only dealt with the operator H. We now embark on studying the 'abstract' operator A, assumed only to equal H in part of space; more specifically, we assume A to satisfy Assumption B.1 with $D = B(4\rho)$ for some $\rho \geq \rho_0$ with $\rho_0 > 0$ some fixed number.

The essential tool in comparing (resolvents of) the operators A and H will be the following lemma, which gives a sort of 'resolvent identity':

Lemma B.13. *For any function $\zeta \in C_0^\infty(D)$, we have*

$$\zeta R(z, A) = R(z, H)\zeta + R(z, H)Z(\zeta)R(z, A) \tag{B.55}$$

with

$$Z(\zeta) = [\sqrt{\alpha^{-1}p^2 + \alpha^{-2}}, \zeta]\,\bar{\zeta}_1 + B$$

with an operator B satisfying

$$\|B\|_1 \leq C_{N,\zeta_1} \left(\frac{\sqrt{\alpha}\beta}{\rho}\right)^N \quad \textit{for all } N \in \mathbb{N}.$$

Here, $\zeta_1 \in C_0^\infty(D)$, such that $\zeta_1\zeta = \zeta$ (see (1) in Assumption B.1). More generally:

$$\zeta R(z, A)^k = R(z, H)^k\zeta + \sum_{j=1}^{k} R(z, H)^j Z(\zeta) R(z, A)^{k-j+1} \quad \forall k \in \mathbb{N}. \tag{B.56}$$

Proof. The proof is by induction; we will start with the induction step, since this will show us, that the formula (B.56) does not rely on the actual form of $Z(\zeta)$: if there is a formula like (B.55), then we also have (B.56), with the same $Z(\zeta)$. Assume the formula (B.56) holds for k.

Then

$$\begin{aligned}\zeta R(z,A)^{k+1} &= \zeta R(z,A)^k R(z,A)\\ &= \Big(R(z,H)^k\zeta + \sum_{j=1}^{k} R(z,H)^j Z(\zeta) R(z,A)^{k-j+1}\Big) R(z,A)\\ &= R(z,H)^k\big(R(z,H)\zeta + R(z,H)Z(\zeta)R(z,A)\big)\\ &\quad + \sum_{j=1}^{k} R(z,H)^j Z(\zeta) R(z,A)^{(k+1)-j+1}\\ &= R(z,H)^{k+1}\zeta + \sum_{j=1}^{k+1} R(z,H)^j Z(\zeta) R(z,A)^{(k+1)-j+1},\end{aligned}$$

the second equality by the induction hypothesis, the third by the induction basis.

Rests to prove the induction basis. Note, that it suffices to prove that for any $u \in \mathcal{D}(A)$ and $v \in \mathcal{D}(H)$, we have

$$\big(\zeta u, Hv\big) - \big(Au, \bar\zeta v\big) = \big(u, Z(\zeta)^* v\big).$$

To prove this equality, notice that by (1) in Assumption B.1, there exists a function $\zeta_1 \in C_0^\infty(D)$, such that $\zeta_1\bar\zeta = \bar\zeta$ and

$$A[\phi, \bar\zeta\psi] = A[\zeta_1\phi, \bar\zeta\psi] + \big(B\,u, v\big)$$

for all $\phi, \psi \in \mathcal{D}[A]$, with an operator B satisfying

$$\|B\|_1 \le C_{N,\zeta_1}\left(\frac{\sqrt{\alpha}\beta}{\rho}\right)^N \qquad \text{for all } N \in \mathbb{N}.$$

Now, $\zeta_1 v \in \mathcal{D}[A]$ by (2) in Assumption B.1, since $v \in \mathcal{D}[H]$, and so, since also $u \in \mathcal{D}[A]$,

$$\begin{aligned}A[u, \bar\zeta v] &= A[u, \bar\zeta(\zeta_1 v)] = A[\zeta_1 u, \bar\zeta(\zeta_1 v)] + \big(B\,u, v\big)\\ &= A[\zeta_1 u, \bar\zeta v] + \big(B\,u, v\big)\end{aligned}$$

This means that

$$\begin{aligned}\big(\zeta u, Hv\big) - \big(Au, \bar\zeta v\big) &= H[\zeta u, v] - A[u, \bar\zeta v]\\ &= H[\zeta u, v] - A[\zeta_1 u, \bar\zeta v] + \big(B\,u, v\big).\end{aligned}$$

By (2) in Assumption B.1, $\bar\zeta v \in \mathcal{D}[A]$, since $\bar\zeta \in C_0^\infty(D)$. Since $\zeta_1\zeta = \zeta$ this means, by (2) in Assumption B.1, that

$$A[\zeta_1 u, \bar\zeta v] = A[\zeta_1 u, \zeta_1(\bar\zeta v)] = H[\zeta_1 u, \zeta_1(\bar\zeta v)] = H[\zeta_1 u, \bar\zeta v]$$

and so

$$\begin{aligned}\big(\zeta u, Hv\big) - \big(Au, \bar\zeta v\big) &= H[\zeta u, v] - H[\zeta_1 u, \bar\zeta v] + \big(B\,u, v\big)\\ &= \big(\zeta u, (\sqrt{\alpha^{-1}p^2 + \alpha^{-2}})\,v\big) - \big(\zeta_1 u, (\sqrt{\alpha^{-1}p^2 + \alpha^{-2}}\,)\,\bar\zeta v\big)\\ &\quad + \big(\zeta u, (V - \alpha^{-1})v\big) - \big(\zeta_1 u, (V - \alpha^{-1})\bar\zeta v\big) + \big(B\,u, v\big)\end{aligned}$$

The last term equals 0, since $\zeta_1\zeta = \zeta$, which leaves us with

$$\begin{aligned}
&\big(\zeta u,(\sqrt{\alpha^{-1}p^2+\alpha^{-2}})\,v\big) - \big(\zeta_1 u,(\sqrt{\alpha^{-1}p^2+\alpha^{-2}}\,)\,\bar\zeta v\big) + \big(B\,u,v\big)\\
&\quad = \big(\zeta\zeta_1 u,(\sqrt{\alpha^{-1}p^2+\alpha^{-2}})\,v\big) - \big(\zeta_1 u,(\sqrt{\alpha^{-1}p^2+\alpha^{-2}}\,)\,\bar\zeta v\big)\\
&\qquad\quad + \big(B\,u,v\big)\\
&\quad = \big(u,\zeta_1\,[\bar\zeta,\sqrt{\alpha^{-1}p^2+\alpha^{-2}}]v\big) + \big(B\,u,v\big)\\
&\quad = \big(u,Z(\zeta)^*v\big)
\end{aligned}$$

with

$$Z(\zeta) = [\sqrt{\alpha^{-1}p^2+\alpha^{-2}},\zeta]\,\bar\zeta_1 + B,$$

with an operator B satisfying

$$\|B\|_1 \le C_{N,\zeta_1}\left(\frac{\sqrt{\alpha}\beta}{\rho}\right)^N \qquad \text{for all } N\in\mathbb{N}.$$

$\square$

The previous lemma will provide us with the tool to study the trace norm of differences of powers of the resolvents of A and H as in the following lemma:

Lemma B.14. *Let the operator A satisfy Assumption B.1 with $D = B(4\rho)$, $\rho\ge\rho_0$. Then for any χ with* $\operatorname{supp}\chi\subset B(\rho)$, $|\chi|\le 1$, *any $k\ge 1$, $K>3$ and $P\ge 1$ integers, we have that*

$$\begin{aligned}
&\big\|\chi\big[R(z,A)^k - R(z,H)^k\big]\big\|_1\\
&\qquad\le C\left(1+\frac{1}{\sqrt{\alpha}}\frac{1}{d_M(z)}\right)\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3\left(\frac{\beta}{\rho}\right)^{2K}\\
&\qquad\qquad\times\left\{\left(\frac{(\,|z|+M\,)^{1/2}}{d_M(z)}\right)^{2K} + \frac{\alpha^P}{d_M(z)}\right\}\frac{1}{|\operatorname{Im}(z)|^k}.
\end{aligned}\tag{B.57}$$

Proof. Let $\eta\in C_0^\infty(\mathbb{R})$, $|\eta|\le 1$, be a monotone function such that

$$\eta(t) = \begin{cases} 1, & |t|\le 2\\ 0, & |t|\ge 3\end{cases}.$$

Denote $\chi_1(x) = \eta(\frac{|x|}{\rho})$ and let $\phi = 1-\chi_1$. Then $\chi\chi_1 = \chi$ and so we get, that

$$\chi\big[R(z,A)^k - R(z,H)^k\big] = \chi\big[\chi_1 R(z,A)^k - R(z,H)^k\chi_1\big] - \chi R(z,H)^k\phi.$$

This means, that we have to prove the bound (B.57) for the two operators

$$\begin{aligned}
T_1 &= \chi\big[\chi_1 R(z,A)^k - R(z,H)^k\chi_1\big]\\
T_2 &= \chi R(z,H)^k\phi.
\end{aligned}$$

The pair of functions χ, ϕ satisfies the condition (B.6) of Lemma B.8 (with $\nu = 2$), and so by that lemma we have, that

$$\begin{aligned}\|T_2\|_1 = \|\chi\, R(z,H)^k\, \phi\|_1 &\le C\, \frac{1}{d_M(z)^k} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \left(\frac{\beta}{\rho}\right)^{2K} \\ &\qquad \times \left\{ \left(\frac{(\,|z| + M\,)^{1/2}}{d_M(z)}\right)^{2K} + \frac{\alpha^P}{d_M(z)} \right\} \\ &\le C \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \left(\frac{\beta}{\rho}\right)^{2K} \\ &\qquad \times \left\{ \left(\frac{(\,|z| + M\,)^{1/2}}{d_M(z)}\right)^{2K} + \frac{\alpha^P}{d_M(z)} \right\} \frac{1}{|\operatorname{Im}(z)|^k}. \end{aligned} \tag{B.58}$$

Remains to prove the bound (B.57) for the operator T_1. Using Lemma B.13 we have, since $\chi_1 \in C_0^\infty(B(4\rho))$, that

$$\begin{aligned} T_1 &= \sum_{j=1}^{k} T_1^{(j)}, \\ T_1^{(j)} &= \chi R(z,H)^j Z(\chi_1) R(z,A)^{k-j+1}, \quad j = 1, \dots k \end{aligned} \tag{B.59}$$

with

$$Z(\chi_1) = [\sqrt{\alpha^{-1}p^2 + \alpha^{-2}}, \chi_1]\, \bar{\zeta}_1 + B$$

for some function $\zeta_1 \in C_0^\infty(B(4\rho))$ (see (1) in Assumption B.1), and with an operator B satisfying

$$\|B\|_1 \le C_{N,\zeta_1} \left(\frac{\sqrt{\alpha}\beta}{\rho}\right)^N \quad \text{for all } N \in \mathbb{N}, \tag{B.60}$$

and so it suffices to prove the bound (B.57) for the operators $T_1^{(j)}$. To this end, note that we have

$$T_1^{(j)} = \tilde{T}_1^{(j)} + B^{(j)}$$

with

$$\begin{aligned} \tilde{T}_1^{(j)} &= \chi R(z,H)^j \left[\frac{1}{\pi} \int_0^\infty R_t C_1 R_t \sqrt{t}\, dt\right] \bar{\zeta}_1 R(z,A)^{k-j+1} \\ B^{(j)} &= \chi R(z,H)^j\, B\, R(z,A)^{k-j+1} \end{aligned}$$

where $C_1 = [\alpha^{-1}p^2, \chi_1]$ and $R_t = (\alpha^{-1}p^2 + \alpha^{-2} + t)^{-1}$ as earlier (see (B.13)).

Firstly, note that by (B.51) and (B.60), we have (choosing N sufficiently large and using (3.1)) the bound

$$\begin{aligned}\|B^{(j)}\|_1 &= \|\chi R(z,H)^j\, B\, R(z,A)^{k-j+1}\|_1 \\ &\le C\,\frac{1}{d_M(z)^j}\left(\frac{\sqrt{\alpha}\beta}{\rho}\right)^N \frac{1}{|\operatorname{Im}(z)|^{k-j+1}} \\ &\le C\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3\left(\frac{\beta}{\rho}\right)^{2K}\frac{\alpha^P}{d_M(z)}\,\frac{1}{|\operatorname{Im}(z)|^k}. \qquad \text{(B.61)}\end{aligned}$$

Next, note also that $\operatorname{supp}\partial_l\chi_1 \subset B(3\rho)\setminus B(2\rho)\subset \mathbb{R}^3\setminus B(2\rho)$. This means, that the supports of the functions χ and $\partial_l\chi_1$, $l=1,2,3$, are separated like required in Lemma B.8 (with $\nu=2$, see condition (B.6)). The idea is to take advantage of this as in the proof of Lemma B.2.

To this end, choose a monotone C^∞- function ζ, $|\zeta|\le 1$, such that

$$\zeta(t) = \begin{cases} 0, & |t|\le 1/3 \\ 1, & |t|\ge 2/3 \end{cases}$$

and define a family of functions, $\varphi_k\in\mathcal{B}(\mathbb{R}^3)$, $k=2,3,\ldots,2N$, by

$$\varphi_k(x) = \zeta\left(\frac{2N}{\rho}\left[|x|-\rho-\frac{\rho(2N-k)}{2N}\right]\right). \qquad \text{(B.62)}$$

This means, that

$$\varphi_k(x) = \begin{cases} 0, & |x|\le \nu_1(k)\rho = \left(1+\frac{(2N-k)+1/3}{2N}\right)\rho \\ 1, & |x|\ge \nu_2(k)\rho = \left(1+\frac{(2N-k)+2/3}{2N}\right)\rho \end{cases}$$

with $\rho<\nu_1(k)\rho<\nu_2(k)\rho<2\rho$ and $\nu_2(k+1)<\nu_1(k)$. That is, $\varphi_{k+1}\nabla\varphi_k=\nabla\varphi_k$ and $\varphi_k\chi=0$, $k=2,\ldots,2N$. Also, $\varphi_2\nabla\chi_1=\nabla\chi_1$.

In this way, $\varphi_2[\alpha^{-1}p^2,\chi_1]=[\alpha^{-1}p^2,\chi_1]$ (see (B.16))) and so

$$\begin{aligned}\tilde{T}_1^{(j)} &= \chi R(z,H)^j\left[\frac{1}{\pi}\int_0^\infty R_t\varphi_2 C_1 R_t\sqrt{t}\,dt\right]\bar{\zeta}_1 R(z,A)^{k-j+1} \\ &= \chi R(z,H)^j\varphi_2\left[\frac{1}{\pi}\int_0^\infty R_t C_1 R_t\sqrt{t}\,dt\right]\bar{\zeta}_1 R(z,A)^{k-j+1} \\ &\quad -\chi R(z,H)^j\left[\frac{1}{\pi}\int_0^\infty R_t C_2 R_t C_1 R_t\sqrt{t}\,dt\right]\bar{\zeta}_1 R(z,A)^{k-j+1}\end{aligned}$$

since $R_t\varphi_2=\varphi_2R_t-R_tC_2R_t$, by (B.14) (here, $C_k=[\alpha^{-1}p^2,\varphi_k]$, $k=2,\ldots,2N$). The first factor in the first term, $\chi R(z,H)^j\varphi_2$, now satisfies the conditions in Lemma B.8 (the condition (B.6), with $\nu=\nu_1(2)\in\,]1,2\,[$), whereas the second term has gained another commutator, C_2. Repeating this procedure, sticking in another φ_m in front of the C_{m-1} in the last term each time, using that $\varphi_m[\alpha^{-1}p^2,\varphi_{m-1}]=[\alpha^{-1}p^2,\varphi_{m-1}]$, we arrive at

$$\tilde{T}_1^{(j)} =$$
$$\Big\{ \sum_{m=2}^{2N} \Big((-1)^m \chi R(z,H)^j \varphi_m \left[\frac{1}{\pi} \int_0^\infty R_t C_{m-1} R_t \cdots R_t C_1 R_t \sqrt{t}\, dt \right] \Big)$$
$$- \chi R(z,H)^j \left[\frac{1}{\pi} \int_0^\infty R_t C_{2N} R_t \cdots R_t C_1 R_t \sqrt{t}\, dt \right] \Big\} \bar{\zeta}_1 R(z,A)^{k-j+1}. \tag{B.63}$$

To estimate the last term in (B.63), note that

$$\begin{aligned} &\|\chi R(z,H)^j \left[\frac{1}{\pi} \int_0^\infty R_t C_{2N} R_t \cdots R_t C_1 R_t \sqrt{t}\, dt \right] \bar{\zeta}_1 R(z,A)^{k-j+1}\| \\ &\le \|\chi R(z,H)^{j-1}\| \, \|\bar{\zeta}_1 R(z,A)^{k-j+1}\| \\ &\quad \times \left\| R(z,H) \left[\frac{1}{\pi} \int_0^\infty R_t C_{2N} R_t \cdots R_t C_1 R_t \sqrt{t}\, dt \right] \right\|_1 \\ &\le \frac{1}{|\operatorname{Im}(z)|^k} \left\| R(z,H) \left[\frac{1}{\pi} \int_0^\infty R_t C_{2N} R_t \cdots R_t C_1 R_t \sqrt{t}\, dt \right] \right\|_1 . \end{aligned}$$

As in the proof of Lemma B.2 (see (B.37)), with

$$Q_l(y) = \left[(q^2+1+y)^{-1/2} q \right] \cdot \left[\nabla \phi_l \, (q^2+1+y)^{-1/2} \right]$$

(with functions $\chi_1, \phi_2, \phi_3 \ldots$) and $\kappa = \alpha\lambda$ for a $\lambda \ge M/\varepsilon$, we get that

$$\begin{aligned} &R(z,H) \frac{1}{\pi} \int_0^\infty R_t C_{2N} R_t \cdots R_t C_1 R_t \sqrt{t}\, dt \\ &= R(-\lambda, H_0)^{1/2} S(\lambda, z) \frac{1}{\pi} \int_0^\infty \alpha^{\frac{5}{2}} (-i\sqrt{\alpha}\beta)^{2N} (\sqrt{q^2+1} - 1 + \kappa)^{-1/2} \\ &\qquad \times (q^2+1+\alpha^2 t)^{-1/2} \Big(\prod_{m=2N}^{1} \{ Q_m(\alpha^2 t) + Q_m(\alpha^2 t)^* \} \Big) \\ &\qquad\quad \times (q^2+1+\alpha^2 t)^{-1/2} \sqrt{t}\, dt. \end{aligned}$$

Now, choosing $\lambda = |z| + M/\varepsilon$, making the change of variables $s = \alpha^2 t$, using the generalised Hölder inequality (3.2), the inequality (3.1) and the bounds (B.22), (B.38) and (B.39) obtained in the proof of Lemma B.2, we get the estimate

$$\begin{aligned} &\|R(z,H) \frac{1}{\pi} \int_0^\infty R_t C_{2N} R_t \cdots R_t C_1 R_t \sqrt{t}\, dt\|_1 \\ &\le C \, \frac{1}{d_M(z)} \left(\frac{\sqrt{\alpha}\beta}{\rho} \right)^{2N-3} \frac{1}{\sqrt{\alpha}} \int_0^\infty (1+s)^{-N+\frac{3}{2}}\, ds. \end{aligned}$$

Choosing $N \ge \max\{K, P + \frac{1}{2}\}$ (note, that $K > 3$, so $N > 3$ and so the s-integral above is convergent) and using that $\alpha \le \alpha_0, \beta \le \beta_0$ and

$\rho \geq \rho_0$, we finally have that

$$\begin{aligned}
&\|\chi R(z,H)^j \left[\frac{1}{\pi}\int_0^\infty R_t C_{2N} R_t \cdots R_t C_1 R_t \sqrt{t}\, dt\right] \bar{\zeta}_1 R(z,A)^{k-j+1}\| \\
&\leq \frac{1}{|\operatorname{Im}(z)^k|} \left\| R(z,H) \left[\frac{1}{\pi}\int_0^\infty R_t C_{2N} R_t \cdots R_t C_1 R_t \sqrt{t}\, dt\right]\right\|_1 \\
&\leq C \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \left(\frac{\beta}{\rho}\right)^{2K} \frac{\alpha^P}{d_M(z)} \frac{1}{|\operatorname{Im}(z)|^k}. \qquad \text{(B.64)}
\end{aligned}$$

The first factor in each of the terms in the sum in (B.63) satisfies the condition (B.6) of Lemma B.8 (with $\nu = \nu_1(k) \in]1,2[$). To estimate the second factor in norm, we apply the same ideas as in the proof of Lemma B.2:

$$\begin{aligned}
&\frac{1}{\pi}\int_0^\infty R_t C_m R_t \cdots R_t C_1 R_t \sqrt{t}\, dt \\
&\qquad = \frac{(-i\sqrt{\alpha}\beta)^m}{\pi\alpha} \int_0^\infty (q^2+1+s)^{-1/2} \\
&\qquad\qquad \times \Big(\prod_{j=m}^{1} \{Q_j(s) + Q_j(s)^*\}\Big) (q^2+1+s)^{-1/2} \sqrt{s}\, ds
\end{aligned}$$

with $Q_j(s)$ as before. By the spectral theorem

$$\begin{aligned}
\|(q^2+1+s)^{-1/2}\| &\leq \frac{1}{\sqrt{1+s}} \\
\|(q^2+1+s)^{-1/2} q_l\| &\leq 1
\end{aligned}$$

and

$$\begin{aligned}
\|Q_j(s)\| &\leq \sum_{l=1}^{3} \|(q^2+1+s)^{-1/2} q_l\| \, \|\partial_l \phi_j\| \, \|(q^2+1+s)^{-1/2}\| \\
&\leq \sum_{l=1}^{3} \|\partial_l \phi_j\| \frac{1}{\sqrt{1+s}}
\end{aligned}$$

(with χ_1 for $j=1$) and so

$$\begin{aligned}
&\left\|\frac{1}{\pi}\int_0^\infty R_t C_m R_t \cdots R_t C_1 R_t \sqrt{t}\, dt\right\| \\
&\qquad \leq \frac{(\sqrt{\alpha}\beta)^m}{\pi\alpha} \Big(\prod_{j=m}^{1}\sum_{l=1}^{3} 2\,\|\partial_l\phi_j\|\Big) \int_0^\infty (1+s)^{-\frac{m+1}{2}}\, ds \\
&\qquad \leq \frac{(\sqrt{\alpha}\beta)^m}{\pi\alpha} \Big(\prod_{j=m}^{1}\sum_{l=1}^{3} 2\,\|\partial_l\phi_j\|\Big) \frac{m+1}{m-1},
\end{aligned}$$

as long as $m > 1$, in order for the integral

$$\int_0^\infty (1+s)^{-\frac{m+1}{2}}\, ds$$

to converge. By construction (see (B.62)),

$$\begin{aligned}\|\partial_l \chi_1\| &\le \frac{1}{\rho}\,\|\eta'\|_\infty,\\ \|\partial_l \phi_j\| &\le \frac{2N}{\rho}\,\|\zeta'\|_\infty, \quad j = 2, \dots, 2N,\end{aligned}$$

and so for $k > 2$, and any $K > 3$, Lemma B.8 finally gives the estimate

$$\begin{aligned}&\|(-1)^k \chi R(z,H)^j \varphi_k \left[\frac{1}{\pi}\int_0^\infty R_t C_{k-1} R_t \cdots R_t C_1 R_t \sqrt{t}\, dt\right] \\ &\qquad\qquad\qquad\qquad\qquad\qquad \times \bar{\zeta}_1 R(z,A)^{k-j+1}\|_1 \\ &\le \frac{C}{d_M(z)^j}\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \left(\frac{\beta}{\rho}\right)^{2K} \left\{\left(\frac{(\,|z| + M\,)^{1/2}}{d_M(z)}\right)^{2K} + \frac{\alpha^P}{d_M(z)}\right\} \\ &\quad \times \left(\frac{\sqrt{\alpha}\beta}{\rho}\right)^{k-1} \frac{1}{\alpha}\frac{1}{|\operatorname{Im}(z)|^{k-j+1}} \\ &\le \frac{C}{d_M(z)}\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \left(\frac{\beta}{\rho}\right)^{2K} \left\{\left(\frac{(\,|z| + M\,)^{1/2}}{d_M(z)}\right)^{2K} + \frac{\alpha^P}{d_M(z)}\right\} \frac{1}{|\operatorname{Im}(z)|^k}\end{aligned} \tag{B.65}$$

since $\alpha \le \alpha_0$, $\beta \le \beta_0$ and $\rho \ge \rho_0$.

We are now left with the term

$$\begin{aligned}&\chi R(z,H)^j \varphi_2 \left[\frac{1}{\pi}\int_0^\infty R_t C_1 R_t \sqrt{t}\, dt\right] \bar{\zeta}_1 R(z,A)^{k-j+1} \\ &\quad = \chi R(z,H)^j \varphi_2 [\sqrt{\alpha^{-1}p^2 + \alpha^{-2}}, \chi_1] \bar{\zeta}_1 R(z,A)^{k-j+1}.\end{aligned}$$

To treat this, we prove the following:

Lemma B.15.

$$\|[\sqrt{\alpha^{-1}p^2 + \alpha^{-2}}, \chi_1]\| \le C\,\frac{\beta}{\sqrt{\alpha}\rho} \tag{B.66}$$

Proof. Note that, by (B.13), (B.14), (B.16), and the change of variables $s = \alpha^2 t$, we have, with $q = \sqrt{\alpha}p = -i\sqrt{\alpha}\beta\nabla$, that

$$\begin{aligned}
&[\sqrt{\alpha^{-1}p^2 + \alpha^{-2}}, \chi_1] \\
&= \sum_{l=1}^{3} \frac{-i\beta}{\pi\sqrt{\alpha}} \int_0^\infty (\alpha p^2 + 1 + s)^{-1} \big((\sqrt{\alpha}p_l)\, \partial_l \chi_1 \\
&\qquad\qquad + \partial_l \chi_1 \,(\sqrt{\alpha}p_l)\big) (\alpha p^2 + 1 + s)^{-1} \sqrt{s}\, ds \\
&= \frac{-i\beta}{\pi\sqrt{\alpha}} \Big\{ \int_0^\infty q(q^2+1+s)^{-2}\sqrt{s}\, ds \;\cdot \nabla\chi_1 \\
&\qquad + \nabla\chi_1 \cdot \int_0^\infty q(q^2+1+s)^{-2}\sqrt{s}\, ds \\
&\qquad + \sum_{l=1}^{3} \Big(\int_0^\infty q_l (q^2+1+s)^{-2} [q^2, \partial_l\chi_1] (q^2+1+s)^{-1} \sqrt{s}\, ds \\
&\qquad\qquad - \int_0^\infty (q^2+1+s)^{-1} [q^2, \partial_l \chi_1] q_l (q^2+1+s)^{-2} \sqrt{s}\, ds \Big) \Big\}.
\end{aligned} \tag{B.67}$$

By the change of variable $s = (q^2+1)y$, using the spectral theorem and the definition of χ_1, $\chi_1(x) = \eta(\frac{|x|}{\rho})$, we get that

$$\begin{aligned}
&\left\| \int_0^\infty q(q^2+1+s)^{-2}\sqrt{s}\, ds \;\cdot \nabla\chi_1 \right\| \\
&\leq \Big(\int_0^\infty (1+y)^{-2}\sqrt{y}\, dy \Big) \sum_{l=1}^{3} \Big(\|(q^2+1)^{-1/2} q_l\| \; \|\partial_l \chi_1\| \Big) \leq \frac{8}{\rho}\, \|\eta'\|_\infty.
\end{aligned}$$

Using (B.16), $\alpha \leq \alpha_0, \beta \leq \beta_0$ and $\rho \geq \rho_0$, we get that

$$\begin{aligned}
&\big\| [q^2, \partial_l \chi_1](q^2+1+s)^{-1} \big\| \\
&\qquad \leq \sqrt{\alpha}\beta \Big(\sum_{j=1}^{3} \|2\partial_j \partial_l \chi_1\| \; \|q_j (q^2+1+s)^{-1}\| \\
&\qquad\qquad + \|\sqrt{\alpha}\beta\Delta(\partial_l\chi_1)\| \; \|(q^2+1+s)^{-1}\| \Big) \\
&\qquad \leq \frac{C}{\rho}\, (1+s)^{-1/2}
\end{aligned}$$

(remember that the derivatives of η are supported in $[2,3]$) and so, since by the spectral theorem

$$\|q_l(q^2+1+s)^{-2}\| \leq (1+s)^{-3/2}$$

we get the estimate

$$\begin{aligned}&\left\|\int_0^\infty q_l(q^2+1+s)^{-2}[q^2,\partial_l\chi_1](q^2+1+s)^{-1}\sqrt{s}\,ds\right\|\\&\leq\frac{C}{\rho}\int_0^\infty(1+s)^{-2}\sqrt{s}\,ds\leq\frac{\tilde{C}}{\rho}.\end{aligned}$$

Noting, that all terms in (B.67) are of the above forms, this proves the bound (B.66) □

Using (3.1), Lemma B.8 and Lemma B.15, we get the bound

$$\begin{aligned}&\|\chi R(z,H)^j\varphi_2[\sqrt{\alpha^{-1}p^2+\alpha^{-2}},\chi_1]\bar{\zeta}_1R(z,A)^{k-j+1}\|_1\\&\quad\leq\frac{C}{d_M(z)}\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3\left(\frac{\beta}{\rho}\right)^{2K}\\&\quad\quad\times\left\{\left(\frac{(\,|z|+M\,)^{1/2}}{d_M(z)}\right)^{2K}+\frac{\alpha^P}{d_M(z)}\right\}\frac{\beta}{\sqrt{\alpha}\rho}\,\frac{1}{|\operatorname{Im}(z)|^k}.\end{aligned}\tag{B.68}$$

Combining the bounds (B.58), (B.61), (B.64), (B.65) and (B.68), and using $\alpha\leq\alpha_0,\beta\leq\beta_0$ and $\rho\geq\rho_0$, we arrive at the estimate

$$\begin{aligned}&\left\|\chi\big[R(z,A)^k-R(z,H)^k\big]\right\|_1\leq\|T_1\|_1+\|T_2\|_1\\&\qquad\leq C\left(1+\frac{1}{\sqrt{\alpha}}\frac{1}{d_M(z)}\right)\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3\left(\frac{\beta}{\rho}\right)^{2K}\\&\qquad\qquad\times\left\{\left(\frac{(\,|z|+M\,)^{1/2}}{d_M(z)}\right)^{2K}+\frac{\alpha^P}{d_M(z)}\right\}\,\frac{1}{|\operatorname{Im}(z)|^k}.\end{aligned}$$

This finally finishes the proof of the lemma. □

The first application of this lemma will be a bound on local traces of functions of the operator A:

Lemma B.16. *Assume that the operator A satisfy Assumption B.1, with $D=B(4\rho)$, $\rho\geq\rho_0$ and let χ satisfy $\operatorname{supp}\chi\subset B(\rho)$, $|\chi|\leq1$. Then for any $g\in C_0^\infty(\mathbb{R})$ and $K>3$ we have that*

$$\|\chi g(A)\|_1\leq C\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3\left(1+(\alpha M)^3+\frac{1}{\sqrt{\alpha}}\left(\frac{\beta}{\rho}\right)^{2K}\right).\tag{B.69}$$

Proof. For $z=iM$ we have, that, for some $k>6$,

$$\begin{aligned}&\|\chi g(A)\|_1\leq\|\chi R(z,A)^k\|_1\|(A-z)^kg(A)\|\\&\quad\leq\|(A-z)^kg(A)\|\Big(\|\chi R(z,H)^k\|_1+\|\chi[R(z,A)^k-R(z,H)^k]\|_1\Big).\end{aligned}$$

Now, by the spectral theorem, ($z=iM$, $g\in C_0^\infty(\mathbb{R})$)

$$\|(A-z)^kg(A)\|\leq C\,M^k.$$

By Lemma B.9, with $2n = k > 6$, the first term in the second factor is bounded by

$$C\, M^{-k} \left(\frac{\rho}{\sqrt{\alpha\beta}} \right)^3 \left(1 + (\alpha M)^3 \right) \tag{B.70}$$

whereas the second term, by Lemma B.14, is bounded by

$$\begin{aligned} C \, &\left(1 + \frac{1}{\sqrt{\alpha}} \frac{1}{d_M(z)} \right) \left(\frac{\rho}{\sqrt{\alpha\beta}} \right)^3 \left(\frac{\beta}{\rho} \right)^{2K} \\ &\qquad\qquad \times \left\{ \left(\frac{(\,|z| + M\,)^{1/2}}{d_M(z)} \right)^{2K} + \frac{\alpha^P}{d_M(z)} \right\} \frac{1}{|\operatorname{Im}(z)|^k} \\ &\qquad \leq C\, M^{-k} \left(\frac{\rho}{\sqrt{\alpha\beta}} \right)^3 \frac{1}{\sqrt{\alpha}} \left(\frac{\beta}{\rho} \right)^{2K} \end{aligned}$$

since $z = iM$, $\alpha \leq \alpha_0$, $\beta \leq \beta_0$ and $\rho \geq \rho_0$. Together with the bound (B.70), this proves the lemma. $\square$

To study the difference $g(A) - g(H)$ we use the following representation for a function of a selfadjoint operator in terms of its resolvent (the formula will be proved in appendix F).

Proposition B.17. *Let $g \in C_0^\infty(\mathbb{R})$. Then for any self adjoint operator B we have, for all $n \geq 2$:*

$$\begin{aligned} g(B) = &\sum_{j=0}^{n-1} \frac{1}{\pi j!} \int_{\mathbb{R}} \partial^j g(\lambda) \operatorname{Im}\left[i^j R(\lambda + i, B) \right] d\lambda \\ &+ \frac{1}{\pi (n-1)!} \int_0^1 \tau^{n-1}\, d\tau \int_{\mathbb{R}} \partial^n g(\lambda) \operatorname{Im}\left[i^n R(\lambda + i\tau, B) \right] d\lambda. \end{aligned} \tag{B.71}$$

Using this on $g(A) - g(H)$ and estimating the resulting differences in resolvents, we arrive at:

Theorem B.18. *Suppose A satisfies Assumption B.1 with $D = B(4\rho)$, $\rho \geq \rho_0$, and that $\operatorname{supp} \chi \subset B(\rho)$, $|\chi| \leq 1$. Let $g \in C^\infty(\mathbb{R})$ be a function such that $g(\lambda) = 0$ for $\lambda \geq \lambda_0$ and such that for some $r \geq 0, L_0 > 0$ fixed, we have, for all $L \geq L_0$, that*

$$|\partial^n g(\lambda)| \leq C_n L^n \langle \lambda \rangle^r \quad , \quad \forall n \in \mathbb{N} \tag{B.72}$$

(here, $\langle \lambda \rangle = (1 + |\lambda|^2)^{1/2}$). Then for any $K > 3$:

$$\left\| \chi \left[g(A) - g(H) \right] \right\|_1 \leq C_K\, L^{2K+3} M^{K+1+r} \left(\frac{\beta}{\rho} \right)^{2K-3} \frac{1}{\alpha^2}. \tag{B.73}$$

The constant C_K does not depend on V, other than on the constant ε in (B.4), nor on χ.

Proof. Let $\lambda \in \mathbb{R}$ and $0 < |\tau| \leq 1$. Denote

$$\delta(\lambda, \tau) = R(\lambda + i\tau, A) - R(\lambda + i\tau, H).$$

Now, since $|\tau| \leq 1 \leq M$, we have, for $\lambda \leq -2M$, that

$$d_M(z) = |z - (-M)| \geq |\lambda| - M \geq \frac{|\lambda|}{2},$$
$$|z| + M = \sqrt{\lambda^2 + \tau^2} + M \leq \frac{\sqrt{5}+1}{2}\,|\lambda|$$

and so

$$\frac{(\,|z| + M\,)^{1/2}}{d_M(z)} \leq \frac{\sqrt{2\sqrt{5}+2}}{\sqrt{|\lambda|}}, \qquad \frac{1}{d_M(z)} \leq \frac{2}{|\lambda|}$$

and for $-2M \leq \lambda \leq \lambda_0$, that

$$d_M(z) \geq |\,\mathrm{Im}(z)| = |\tau|, \quad |z| + M \leq C_{\lambda_0} M, \quad C_{\lambda_0} = \sqrt{5 + \lambda_0^2} + 1.$$

Then, by Lemma B.14, with $k = 1$, we have, for any $K > 3$, that

$$\begin{aligned}\|\chi\delta(\lambda,\tau)\|_1 \leq C &\left(1 + \frac{1}{\sqrt{\alpha}}\frac{1}{|\tau|}\right)\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3\left(\frac{\beta}{\rho}\right)^{2K} \\ &\times\left\{\frac{M^K}{|\tau|^{2K}} + \frac{\alpha^P}{|\tau|}\right\}\frac{1}{|\tau|} \qquad -2M \leq \lambda \leq \lambda_0\end{aligned} \tag{B.74}$$

$$\begin{aligned}\|\chi\delta(\lambda,\tau)\|_1 \leq C &\left(1 + \frac{1}{\sqrt{\alpha}}\frac{1}{|\lambda|}\right)\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3\left(\frac{\beta}{\rho}\right)^{2K} \\ &\times\left\{\frac{1}{|\lambda|^K} + \frac{\alpha^P}{|\lambda|}\right\}\frac{1}{|\tau|} \qquad \lambda \leq -2M.\end{aligned} \tag{B.75}$$

Note, that the representation in Proposition B.17 does strictly speaking not apply to the function g, since this is not of compact support. In order to correct this, we use the fact, that $H \geq -M$, $A \geq -\alpha^{-1}$ (see (3) in Assumption B.1) and modify g: Let $\zeta \in C^\infty(\mathbb{R})$ be a monotone function such that $\zeta(t) = 0, t \leq -2$ and $\zeta(t) = 1, t \geq -3/2$. Define then, with $\tilde{M} = \max\{M, \alpha^{-1}\}$, the function $\tilde{g} \in C_0^\infty(\mathbb{R})$ by

$$\tilde{g}(\lambda) = \zeta(\frac{\lambda}{\tilde{M}})\, g(\lambda).$$

Since $H \geq -\tilde{M}$, $A \geq -\tilde{M}$ and $\tilde{g}(\lambda) = g(\lambda)$ for $\lambda \geq -\frac{3}{2}\tilde{M}$, we have, by the spectral theorem, that $\tilde{g}(A) = g(A)$ and $\tilde{g}(H) = g(H)$. Note also, that by (B.72), and since $L \geq L_0$,

$$|\partial^n \tilde{g}(\lambda)| \leq \tilde{C}_n L^n \langle\lambda\rangle^r \quad , \quad \forall n \in \mathbb{N} \tag{B.76}$$

with constants $\tilde{C}_n$ depending on the C_j's ($j \leq n$) in (B.72), on L_0, and the derivatives of ζ but not on the lower bounds, $-M$ of H and $-\alpha^{-1}$ of A, since $\tilde{M} \geq M \geq 1$. Then, by the representation (B.71) we get

$$\tilde{g}(A) - \tilde{g}(H) = I_1^{(n)} + I_2^{(n)} \qquad \forall n \in \mathbb{N}$$

with

$$I_1^{(n)} = \sum_{j=0}^{n-1} \frac{1}{\pi j!} \int_{\mathbb{R}} \partial^j \tilde{g}(\lambda)\, \mathrm{Im}\left[i^j \delta(\lambda,1)\right] d\lambda$$

$$I_2^{(n)} = \frac{1}{\pi(n-1)!} \int_0^1 \tau^{n-1}\, d\tau \int_{\mathbb{R}} \partial^n \tilde{g}(\lambda)\, \mathrm{Im}\left[i^n \delta(\lambda,\tau)\right] d\lambda$$

where the integration in λ in fact only takes places over the interval $[-2\tilde{M}, \lambda_0]$.

To estimate $\chi I_2^{(n)}$, choose $n = 2K+3$. Using the estimates (B.74), (B.75) and (B.76), and the fact that $\alpha \le \alpha_0$, $\beta \le \beta_0$, $M \ge 1$, and $|\tau| \le 1$ on the domain of integration, we get

$$\begin{aligned} \|\chi I_2^{(n)}\|_1 \le C\, L^{2K+3} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \left(\frac{\beta}{\rho}\right)^{2K} \\ \Big\{ \int_0^1 \tau^{2K+1}\, d\tau \int_{-2\tilde{M}}^{-2M} \Big(1 + \frac{1}{\sqrt{\alpha}} \frac{1}{|\lambda|}\Big)\Big(\frac{1}{|\lambda|^K} + \frac{\alpha^P}{|\lambda|}\Big) |\lambda|^r\, d\lambda \\ + \int_0^1 d\tau \int_{-2M}^{\lambda_0} \frac{M^{K+r}}{\sqrt{\alpha}}\, d\lambda \Big\}. \end{aligned}$$

(Note, that $|\lambda|^r \le C(\lambda_0)\, M^r$ for $-2M \le \lambda \le \lambda_0$, since $M \ge 1$). Now, again using that $\tilde{M} = \max\{M, \alpha^{-1}\}$, $\alpha \le \alpha_0$ and $M \ge 1$, we have, for $r > 0$, that

$$\begin{aligned} \int_{-2\tilde{M}}^{-2M} \Big(1 + \frac{1}{\sqrt{\alpha}} \frac{1}{|\lambda|}\Big)\Big(\frac{1}{|\lambda|^K} + \frac{\alpha^P}{|\lambda|}\Big) |\lambda|^r\, d\lambda \\ \le \frac{C}{\sqrt{\alpha}} \int_M^{\tilde{M}} \left(\frac{1}{\lambda^K} + \frac{\alpha^P}{\lambda}\right) \lambda^r\, d\lambda \\ \le \frac{C}{\sqrt{\alpha}} \Big(\alpha^{K-r-1} - M^{-K+r+1} + \alpha^{P-r}\Big) \le \frac{C}{\sqrt{\alpha}} M^{K+1+r} \end{aligned}$$

since $\tilde{M} = \max\{M, \alpha^{-1}\}$, $\alpha \le \alpha_0$ and $M \ge 1$. For $r = 0$, we get $-\alpha^P \log \alpha$ instead of α^{P-r}, which is positive and also bounded above for $\alpha \in]0,1]$.

In this way,

$$\|\chi I_2^{(n)}\|_1 \le C\, L^{2K+3} M^{K+1+r} \left(\frac{\beta}{\rho}\right)^{2K-3} \frac{1}{\alpha^2}. \tag{B.77}$$

By the same estimates we have (since $L \geq L_0$), that (recall, that $n = 2K+3$)

$$\begin{aligned}
\|\chi I_1^{(n)}\|_1 \leq C\, L^{2K+2} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \left(\frac{\beta}{\rho}\right)^{2K} \\
\Big\{ \int_{-\tilde{2}M}^{-2M} \left(1 + \frac{1}{\sqrt{\alpha}}\frac{1}{|\lambda|}\right)\left(\frac{1}{|\lambda|^K} + \frac{\alpha^P}{|\lambda|}\right) |\lambda|^r \, d\lambda \\
+ \int_{-2M}^{\lambda_0} \frac{M^{K+r}}{\sqrt{\alpha}}\, d\lambda \Big\} \\
\leq C\, L^{2K+3} M^{K+1+r} \left(\frac{\beta}{\rho}\right)^{2K-3} \frac{1}{\alpha^2}.
\end{aligned} \tag{B.78}$$

Notice, that we can assume throughout, that $\tilde{M} = \alpha^{-1}$ when dealing with the integrals over $\lambda \in [-2\tilde{M}, -2M]$, since otherwise $\tilde{M} = M$ and hence the integrals are zero; this also means, that $\alpha \leq 1$ (in this case), since $M \geq 1$.

Now, the estimates (B.77) and (B.78) provides the bound (B.73), which finishes the proof of the theorem. □

Finally, we use the technique from the proof of this theorem, and the estimate (B.8) from Lemma B.2, to prove the following bound on $\|\chi\, g(H)\, \phi\|_1$:

Theorem B.19. *Let the functions χ and ϕ satisfy (B.6) for $\rho \geq \rho_0$, and let H be as in (B.1), with a potential satisfying (B.4) for $X = |V|^{1/2}$. Let $g \in C^\infty(\mathbb{R})$ be a function such that $g(\lambda) = 0$ for $\lambda \geq \lambda_0$ and such that for some $r \geq 0, L_0 > 0$ fixed, we have, for all $L \geq L_0$, that*

$$|\partial^n g(\lambda)| \leq C_n L^n \langle\lambda\rangle^r \quad , \quad \forall n \in \mathbb{N} \tag{B.79}$$

(here, $\langle\lambda\rangle = (1+|\lambda|^2)^{1/2}$). Then, for any $K > 3$

$$\|\chi\, g(H)\, \phi\|_1 \leq C_K\, L^{2K+2} M^{K+1+r} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \left(\frac{\beta}{\rho}\right)^{2K}. \tag{B.80}$$

The constant C_K does not depend on V, other than on the constant ε in (B.4), nor on χ.

Proof. This goes as the proof of Theorem B.18; we again note that in order to use the representation (B.71) we need to modify the function g, since this is not of compact support: Let ζ be the function from the proof of Theorem B.18, and define $\tilde{g}(\lambda) = \zeta(\frac{\lambda}{M})g(\lambda)$, then $\tilde{g}(H) = g(H)$ by the spectral theorem, since $H \geq -M$ by (B.4). Again, $\tilde{g}$ satisfies estimates like (B.79), with constants only depending on L_0, the C_j's ($j \leq n$) from (B.79), and the derivatives of the function ζ. Now, since $\tilde{g}(\lambda) = 0$ for $\lambda \leq -2M$, we only need the following:

$$-2M \leq \lambda \leq \lambda_0 \quad \Rightarrow \quad d_M(z) \geq |\tau|, \quad |z| + M \leq C_{\lambda_0} M.$$

Using this, and (B.8), we have, for all $K > 3$, that

$$\|\chi\, R(\lambda + i\tau, H)\, \phi\|_1 \le C \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \left(\frac{\beta}{\rho}\right)^{2K} \frac{1}{|\tau|}\left\{\frac{M^K}{|\tau|^{2K}} + \frac{\alpha^P}{|\tau|}\right\} \quad -2M \le \lambda \le \lambda_0. \tag{B.81}$$

Applying the representation (B.71), with $n = 2K + 2$, to the operator H, using the estimates (B.79) and (B.81) (and that $L \ge L_0$, $\alpha \le \alpha_0$), we get that (since $\tilde{g}$ and all its derivatives vanish for $\lambda \le -2M$)

$$\begin{aligned}\|\chi\, R(\lambda + i\tau, H)\, \phi\|_1 &\le C\, L^{2K+2} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \left(\frac{\beta}{\rho}\right)^{2K} \\ &\quad \times \left[\int_{-2M}^{\lambda_0} M^{K+r}\, d\lambda + \int_0^1 d\tau \int_{-2M}^{\lambda_0} M^{K+r}\, d\lambda\right]. \\ &\le C\, L^{2K+2} M^{K+1+r} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \left(\frac{\beta}{\rho}\right)^{2K}.\end{aligned}$$

This proves the theorem. $\square$

We finish this appendix by proving a result on the non-locality of the operator

$$H_0 = \sqrt{-\alpha^{-1}\beta^2\Delta + \alpha^{-2}} - \alpha^{-1}.$$

As ususal, $\alpha \in]0, \alpha_0]$ and $\beta \in]0, \beta_0]$ for some fixed α_0, $\beta_0 > 0$. We prove this result here, since it utilizes the techniques developed in this appendix; it also (partly) explains the reason for Assumption B.1.

Proposition B.20. *Let $\chi \in C_0^\infty(B(\rho))$ for some $\rho \ge \rho_0$ with $\rho_0 > 0$ fixed, and let ϕ be a function such that* $\operatorname{supp}\phi \subset \mathbb{R}^3 \setminus B(\nu\rho)$ *for some $\nu > 1$. Then for all $K \ge 1$ there exists a constant C_K such that*

$$\|\phi H_0 \chi\|_1 \le C_K \left(\frac{\sqrt{\alpha}\beta}{\rho}\right)^K. \tag{B.82}$$

Proof. We use the representation from Lemma B.3 (with $p = -i\beta\nabla$ and $R_t = (\alpha^{-1}p^2 + \alpha^{-2} + t)^{-1}$ as usual):

$$\begin{aligned}\phi H_0 \chi &= \phi\Big(-\frac{1}{\pi}\int_0^\infty \big((\alpha^{-1}p^2 + \alpha^{-2} + t)^{-1} - t^{-1}\big)\sqrt{t}\, dt\Big)\chi \\ &= \phi\Big(-\frac{1}{\pi}\int_0^\infty (\alpha^{-1}p^2 + \alpha^{-2} + t)^{-1}\sqrt{t}\, dt\Big)\chi \\ &= \phi\Big(\frac{1}{\pi}\int_0^\infty R_t[\alpha^{-1}p^2, \chi]R_t\sqrt{t}\, dt\Big)\end{aligned} \tag{B.83}$$

since $\phi\chi = 0$. Using that also $\phi[\alpha^{-1}p^2, \chi] = 0$ (see (B.16)), we have that (B.83) equals

$$\phi\Big(\frac{1}{\pi}\int_0^\infty [R_t,[\alpha^{-1}p^2,\chi]]R_t\sqrt{t}\,dt\Big)$$
$$= \phi\Big(-\frac{1}{\pi}\int_0^\infty R_t[\alpha^{-1}p^2,[\alpha^{-1}p^2,\chi]]R_t^2\sqrt{t}\,dt\Big).$$

Continuing this way, we arrive at

$$\begin{aligned}
&\phi H_0\chi \\
&= \phi\,\Big(\frac{(-1)^{N-1}}{\pi}\int_0^\infty R_t\,\underbrace{[\alpha^{-1}p^2,[\alpha^{-1}p^2,[\dots[\alpha^{-1}p^2,\chi]\dots]]]}_{N\times\alpha^{-1}p^2}\,R_t^N\sqrt{t}\,dt\Big) \\
&= \phi\,\Big(\frac{(-1)^{N-1}}{\alpha\pi}\int_0^\infty \tilde{R}_s\,\underbrace{[q^2,[q^2,[\dots[q^2,\chi]\dots]]]}_{N\times q^2}\,\tilde{R}_s^N\sqrt{s}\,ds\Big) \qquad \text{(B.84)}
\end{aligned}$$

with $\tilde{R}_s = (q^2+1+s)^{-1}$, $q = -i\sqrt{\alpha}\beta\nabla$, by the change of variables $s = \alpha^2 t$. To proceed, we prove the following:

Lemma B.21. *For all N, with $q = -i\sqrt{\alpha}\beta\nabla$:*

$$\underbrace{[q^2,[q^2,[\dots[q^2,\chi]\dots]]]}_{N\times q^2} = \big(-i\sqrt{\alpha}\beta\big)^N \sum_{\substack{|\eta|+|\gamma|=2N\\ |\eta|\le N}} a(\eta,\gamma)\,(\partial^\gamma\chi)\,q^\eta. \tag{B.85}$$

for some constants $a(\eta,\gamma)$, depending also on α and β, but bounded for $\alpha \in\,]0,\alpha_0]$ and $\beta \in\,]0,\beta_0]$.

Proof. Goes by induction: For $N = 1$, by (B.16):

$$\begin{aligned}
[q^2,\chi] &= -i\sqrt{\alpha}\beta\big(2\nabla\chi\cdot q - i\sqrt{\alpha}\beta\Delta\chi\big) \\
&= (-i\sqrt{\alpha}\beta)\sum_{l=1}^{3}\Big\{2\,(\partial_l\chi)\,q_l + (-i\sqrt{\alpha}\beta)\,\partial_l^2\chi\Big\}
\end{aligned}$$

which is of the form (B.85).

Assume that the formula (B.85) holds for some N. Then

$$\underbrace{[q^2,[q^2,[\dots[q^2,\chi]\dots]]]}_{(N+1)\times q^2} = \big(-i\sqrt{\alpha}\beta\big)^N \sum_{\substack{|\eta|+|\gamma|=2N\\ |\eta|\le N}} a(\eta,\gamma)[q^2,(\partial^\gamma\chi)\,q^\eta]$$

Now, an easy computation, using (B.16), yields that

$$\begin{aligned}
&[q^2,(\partial^\gamma\chi)\,q^\eta] \\
&\quad = \sum_{l=1}^{3}\Big\{2(-i\sqrt{\alpha}\beta)(\partial_l\partial^\gamma\chi)\,q_l q^\eta + (-i\sqrt{\alpha}\beta)^2(\partial_l^2\partial^\gamma\chi)\,q^\eta\Big\}.
\end{aligned}$$

Since $|\eta| + |\gamma| = 2N$ and $|\eta| \leq N$ by the induction hypothesis, this proves that

$$\underbrace{[q^2, [q^2, [\dots[q^2, \chi]\dots]]]}_{(N+1)\times q^2}$$

is of the form

$$\big(-i\sqrt{\alpha}\beta\big)^{N+1} \sum_{\substack{|\tilde\eta|+|\tilde\gamma|=2(N+1)\\ |\tilde\eta|\leq N+1}} \tilde a(\tilde\eta, \tilde\gamma)\,(\partial^{\tilde\gamma}\chi)\, q^{\tilde\eta}.$$

The lemma now follows by induction. □

We wish to use the following (see Reed and Simon [25, Thm. XI.21 p. 47]:

Lemma B.22. *Define*

$$L^2_\delta(\mathbb{R}^3) = \big\{ f \;\big|\; \|f\|_\delta \equiv \|(1+x^2)^{\delta/2} f(x)\|_{L^2(\mathbb{R}^3)} < \infty \big\}.$$

Suppose $f, g \in L^2_\delta(\mathbb{R}^3)$ for some $\delta > 3/2$. Then $f(x)g(-i\nabla)$ is a trace class operator and

$$\|f(x)g(-i\nabla)\|_1 \leq c_\delta \|f\|_\delta \|g\|_\delta.$$

Remark B.23. By scaling this means, that for $h \in]0, h_0]$:

$$\|f(x)g(-ih\nabla)\|_1 \leq c_{\delta,h_0} h^{-\frac{3}{2}-\delta} \|f\|_\delta \|g\|_\delta \tag{B.86}$$

with $c_{\delta,h_0} = c_\delta(1+h_0^2)^{\delta/2}$; compare also with Lemma B.4.

Indeed, with $\delta = 3/2 + \epsilon$, $\epsilon > 0$, we have that (remember that $|\eta| \leq N$)

$$\begin{aligned}
\|q^\eta \tilde R_s^N\|_\delta^2 = \|(1+q^2)^{\delta/2} q^\eta \tilde R_s^N\|^2_{L^2(\mathbb{R}^3)} &= \int_{\mathbb{R}^3} \frac{(1+q^2)^{3+2\epsilon} q^{2\eta}}{(q^2+1+s)^{2N}}\, d^3q \\
&\leq 4\pi(1+s)^{-N+\frac{9}{2}+2\epsilon}\, 2^{3+2\epsilon}\Big(1 + \int_1^\infty t^{8+4\epsilon-2N}\, dt\Big).
\end{aligned}$$

by the change of variables $q = (\sqrt{1+s})x$ $(t = |x|)$. Choosing $\epsilon < 3/4$ (so that $\delta < 9/4$) and $N \geq 7$, this gives us that

$$\|q^\eta \tilde R_s^N\|_\delta^2 \leq 96\sqrt{2}\,\pi(1+s)^{-N+6}$$

In this way, choosing $N \geq 8$ and remembering that $\epsilon < 3/4$, using (3.1), and that $\|\tilde R_s\| \leq (1+s)^{-1}$ by the spectral theorem, we have, by

(B.86) that (remember that $q = -i\sqrt{\alpha}\beta\nabla$)

$$
\begin{aligned}
&\left\| \int_0^\infty \tilde{R}_s(\partial^\gamma \chi)\, q^\eta \tilde{R}_s \sqrt{s}\, ds \right\|_1 \\
&\le c(\delta, \alpha_0, \beta_0) \left(\sqrt{\alpha}\beta\right)^{-3-\frac{3}{4}} \int_0^\infty \|\tilde{R}_s\|\, \|\partial^\gamma \chi\|_\delta \|q^\eta \tilde{R}_s^N\|_\delta \sqrt{s}\, ds \\
&\le\; C\, \left(\sqrt{\alpha}\beta\right)^{-3-\frac{3}{4}} \|\partial^\gamma \chi\|_\delta \int_0^\infty (1+s)^{-\frac{N}{2}+3} \frac{\sqrt{s}\, ds}{1+s} \\
&\le\; C'\, \left(\sqrt{\alpha}\beta\right)^{-3-\frac{3}{4}} \|\partial^\gamma \chi\|_\delta
\end{aligned}
$$

Remember, that $|\gamma| \ge N$ and that $\chi \in C_0^\infty(B(\rho))$, so that, since $\delta \le 9/4$,

$$
\|\partial^\gamma \chi\|_\delta \le \|\partial^\gamma \chi\|_{9/4} = \|(1+x^2)^{9/4} \partial^\gamma \chi(x)\|_{L^2(\mathbb{R}^3)} \le C\, \rho^{\frac{15}{4}-N},
$$

and so

$$
\left\| \int_0^\infty \tilde{R}_s(\partial^\gamma \chi)\, q^\eta \tilde{R}_s \sqrt{s}\, ds \right\|_1 \le C\, \left(\sqrt{\alpha}\beta\right)^{-3-\frac{3}{4}} \rho^{\frac{15}{4}-N}.
$$

Finally, given $K \ge 1$, let $N = K + 7 \ge 8$; then the above shows that, by Lemma B.21 and (B.84),

$$
\begin{aligned}
&\|\phi H_0 \chi\|_1 \\
&\le \|\phi\|_\infty \frac{(\sqrt{\alpha}\beta)^N}{\alpha\pi} \sum_{\substack{|\eta|+|\gamma|=2N \\ |\eta|\le N}} |a(\eta,\gamma)|\, \left\| \int_0^\infty \tilde{R}_s \partial^\gamma \chi\, q^\eta \tilde{R}_s^N \sqrt{s}\, ds \right\|_1 \\
&\le \frac{\tilde{C}}{\alpha}\, \left(\sqrt{\alpha}\beta\right)^{K+7-3-\frac{3}{4}} \left(\frac{1}{\rho}\right)^{K+7-\frac{15}{4}} \le C_K\, \left(\frac{\sqrt{\alpha}\beta}{\rho}\right)^K
\end{aligned}
$$

since $\alpha \in]0, \alpha_0]$, $\beta \in]0, \beta_0]$ and $\rho \ge \rho_0$ for some fixed $\alpha_0,\ \beta_0, \rho_0 > 0$. This finishes the proof of the proposition. □

Appendix C. Reduction to Asymptotic Potential

The aim of this section is to study the reduction to the operator

$$
H_W = \sqrt{\alpha^{-1} p^2 + \alpha^{-2}} - \alpha^{-1} + W(x)
$$

with the potential $W(x)$, being the asymptotic part of the potential V as $|x| \to \infty$, instead of the full potential $V(x)$. Concretely, one should think of

$$
V(x) = -\frac{\delta}{|x|} + \rho_{TF,\delta} * |x|^{-1} \tag{C.1}
$$

where $\rho_{TF,\delta}$ is the Thomas-Fermi density for an atom with nuclear charge δ (see Lieb and Simon [21]; see also Lieb [19, 20]); one has, that $\rho_{TF,\delta} * |x|^{-1}$ is continuous (even at $|x| = 0$).

The idea of this study is, that when treating the many-body problem, one starts by eliminating the electron-electron interaction, by replacing it by an effective potential (plus an error). This effective potential will later play the rôle of V, whereas its asymptotic behaviour will be that of the Coulomb potential,

$$W(x) = -\frac{\delta}{|x|}. \tag{C.2}$$

In this thesis we shall only use this analysis on a more trivial case though, see the proof of Theorem 7.4.

The idea is to show that, under suitable conditions, we can replace H_V in the trace $\mathrm{Tr}\{\psi\, g(H_V)\}$ by the operator H_W, modulo errors. This result, and the techniques to obtain it, are closely related to that of the previous section, when replacing the abstract operator A with the operator H_V. At the end of this section, we shall put these two results together, to compare $\mathrm{Tr}\{\psi\, g(A)\}$ with $\mathrm{Tr}\{\psi\, g(H_W)\}$.

The general conditions on the two potentials W and V will be the following: Assume that both $X = |W|^{1/2}$ and $X = |V|^{1/2}$ satisfy:

$$\|Xu\|^2 \le \varepsilon(H_0 u, u) + M(\beta,\varepsilon)\|u\|^2 \quad \text{for all } u \in C_0^\infty(\mathbb{R}^3) \tag{C.3}$$

for some $M = M(\beta,\varepsilon)$ and a fixed $\varepsilon \in]0,1[$. Note, that we can assume $|W|^{1/2}$ and $|V|^{1/2}$ to satisfy the above with the same ε and $M(\beta,\varepsilon)$; we can also assume, without restriction, that $M = M(\beta,\varepsilon) \ge 1$. This means, that both H_V and H_W are bounded from below by $-M(\beta,\varepsilon)$, and we can therefore define their Friedrichs-extensions, to get two self adjoint operators in $L^2(\mathbb{R}^3)$. By abuse of notation, we shall also denote these two operators by H_V and H_W.

Secondly, we express, that W is the asymptotic form of V, as $|x| \to \infty$, as follows: We assume, that we have real-valued functions $\Psi \in L^\infty(\mathbb{R}^3)$, $F \in L^\infty_{\mathrm{loc}}(\mathbb{R}^3)$ and Y satisfying (C.3), such that, for some $\rho > 0$

$$\left.\begin{aligned} W(x) &= Y(x)\Psi(x)Y(x) \\ V(x) &= Y(x)(\Psi(x)+F(x))Y(x) \end{aligned}\right\} \quad \text{for } x \in B(\rho). \tag{C.4}$$

Remark C.1. Not, that the potentials V from (C.1) and W from (C.2) satisfy this.

The starting point is, as in the last section, to study the resolvents of the two involved operators, H_W and H_V. To this end, note the following:

Lemma C.2. *For all $\phi \in \mathcal{B}^\infty(\mathbb{R}^3)$ we have that*

$$\phi R(z,H_V) = R(z,H_W)\phi + R(z,H_W)Z_1(\phi)R(z,H_V) \tag{C.5}$$

where

$$Z_1(\phi) = [\sqrt{\alpha^{-1}p^2 + \alpha^{-2}}, \phi] + \phi F Y^2. \tag{C.6}$$

More generally,

$$\phi R(z,H_V)^k = R(z,H_W)^k\phi + \sum_{j=1}^{k} R(z,H_W)^j Z_1(\phi) R(z,H_V)^{k-j+1}, \forall k\in\mathbb{N}. \quad \text{(C.7)}$$

Proof. Note first, that the induction proof of the similar result, Lemma B.13, does not rely on the exact expression for $Z_1(\phi)$; this means, that all we have to prove is (C.5). It suffices to prove, that

$$\big(\phi u, H_V v\big) - \big(H_W u, \bar\phi v\big) = \big(u, Z_1^*(\phi)v\big) \quad \forall u\in\mathcal{D}(H_W),\ v\in\mathcal{D}(H_V).$$

This follows from an easy computation. □

Next, let $|f|_\rho = \sup_{|x|\le\rho}|f(x)|$ be the supremums-norm of $f\in L^\infty_{\mathrm{loc}}(\mathbb{R}^3)$ in the ball of radius $\rho>0$, and let, for F in (C.4),

$$K(z,\rho) = (\,|z|+M\,)|F|_\rho. \quad \text{(C.8)}$$

Also, throughout this section, we assume that $\rho\ge\rho_0$ for some fixed $\rho_0>0$. We now prove a result similar to Lemma B.14 of the pair of operators A and H_V:

Lemma C.3. *Let V and W be as defined above, with some $\rho\ge\rho_0$. Then for any function χ, with $\operatorname{supp}\chi\subset B(\rho/2)$, $|\chi|\le 1$, and any integers $N\ge 1$ and $P\ge 1$:*

$$\begin{aligned}\big\|\chi\big[R(z,H_V)-R(z,H_W)\big]\big\| &\le \frac{C_N}{d_M(z)}\left(1+\frac{1}{\sqrt{\alpha}}\frac{1}{d_M(z)}\right)\left(\frac{\beta}{\rho}\right)^N \\ &\quad\times\left\{\left(\frac{(\,|z|+M\,)^{1/2}}{d_M(z)}\right)^N + \frac{\alpha^P}{d_M(z)}\right\} \quad + \quad \frac{K(z,\rho)}{d_M(z)^2}.\end{aligned} \quad \text{(C.9)}$$

If $k>14$ then for any $K>3$

$$\begin{aligned}\big\|\chi[R(\pm iM,H_V)^k - R(\pm iM,H_W)^k]\big\|_1 &\le C_K\,M^{-k}\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3\left\{\left(\frac{\beta}{\rho}\right)^{2K}\left(\frac{1}{M^K}+\frac{\alpha^P}{M}\right)\left(1+\frac{1}{\sqrt{\alpha}}\frac{1}{M}\right)\right. \\ &\quad \left. + \frac{K(0,\rho)}{M}\big(1+(\alpha M)^3\big)\right\}.\end{aligned} \quad \text{(C.10)}$$

The constants C_N and C_K do not depend on V, W, χ or ρ.

Proof. The idea of the proof is very reminiscent of that of Lemma B.14: Choose a monotone function $\eta\in C_0^\infty(\mathbb{R})$, $|\eta|\le 1$, such that

$$\eta(t) = \begin{cases} 1, & |t|\le\frac{2}{3} \\ 0, & |t|\ge 1\end{cases}.$$

Letting $\chi_1(x) = \eta(\frac{|x|}{\rho})$ and $\phi = 1 - \chi_1$, we have, that

$$\begin{aligned}\chi[R(z,H_V)^k - R(z,H_W)^k]&\\ &= \chi[\chi_1 R(z,H_V)^k - R(z,H_W)^k \chi_1] - \chi R(z,H_W)^k \phi\end{aligned} \tag{C.11}$$

since $\chi_1 = 1$ on $\operatorname{supp}\chi$. This means that we have to prove the bounds (C.9) (with $k = 1$) and (C.10) for the operators

$$\begin{aligned}T_1 &= \chi[\chi_1 R(z,H_V)^k - R(z,H_W)^k \chi_1]\\ T_2 &= \chi R(z,H_W)^k \phi.\end{aligned}$$

The estimate (C.10) is satisfied by the operator T_2, due to Lemma B.8 (with $z = \pm iM$), since $\operatorname{dist}\{\operatorname{supp}\chi, \operatorname{supp}\phi\} \geq \frac{1}{6}\rho$. (Note, that Lemma B.8 did not use the form of the potential W, only that it satisfies the condition (C.3)).

As for the operator T_1, we use the same idea as in the proof of Lemma B.14, namely to apply the 'resolvent identity' (C.7), to get the identity

$$\begin{aligned}T_1 &= \sum_{j=1}^{k} T_1{}^{(j)}\\ T_1^{(j)} &= \chi R(z,H_W)^j Z_1(\chi_1) R(z,H_V)^{k-j+1} \quad , \quad j = 1,\ldots k,\end{aligned}$$

with

$$Z_1(\chi_1) = [\sqrt{\alpha^{-1}p^2 + \alpha^{-2}}, \chi_1] + \chi_1 F Y^2.$$

Let $\chi_2(x) = \eta(\frac{|x|}{2\rho})$. Then $\chi_1\chi_2 = \chi_1$, and so

$$\begin{aligned}&\|T_1{}^{(j)}\|_1\\ &= \|\chi R(z,H_W)^j \left\{[\sqrt{\alpha^{-1}p^2 + \alpha^{-2}}, \chi_1] + \chi_1\chi_2 F Y^2\right\} R(z,H_V)^{k-j+1}\|_1\\ &\leq \|\chi R(z,H_W)^j [\sqrt{\alpha^{-1}p^2 + \alpha^{-2}}, \chi_1] R(z,H_V)^{k-j+1}\|_1\\ &\quad + \|\chi R(z,H_W)^j \chi_1 F Y \chi_2 Y R(z,H_V)^{k-j+1}\|_1.\end{aligned} \tag{C.12}$$

For $j \leq k/2$, we have that $k - j > 6$, since $k > 14$, and using (3.1),

$$\begin{aligned}\|\chi R(z,H_W)^j \chi_1 F Y \chi_2 Y R(z,H_V)^{k-j+1}\|_1&\\ &\leq \|\chi R(z,H_W)^j \chi_1 F Y\| \, \|Y \chi_2 R(z,H_V)^{k-j+1}\|_1.\end{aligned}$$

The last factor is (with $z = \pm iM$), by Lemma B.12 (since $k - j > 6$ and the function Y satisfies (C.3)), bounded by

$$C\, M^{-k+j-\frac{1}{2}} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \big(1 + (\alpha M)^3\big).$$

The first factor is, by Lemma B.6, bounded by (recall that $z = \pm iM$)

$$\begin{aligned}\|R(z,H_W)^j\chi_1 Y\| \cdot \Big(\sup_{x\in \operatorname{supp}\chi_1} |F(x)| \quad \Big) \\ &\le \|R(z,H_W)^{j-1}\| \, \|R(z,H_W)\chi_1 Y\| \, |F|_\rho \\ &\le C\, M^{-j+1} M^{-\frac12}\, |F|_\rho = C\, M^{-j+\frac12}\, |F|_\rho.\end{aligned}$$

All in all, recalling (C.8):

$$K(z,\rho) = (\,|z| + M\,)|F|_\rho$$

we get, that for $j \le k/2$, the last term in (C.12) is bounded by

$$\begin{aligned}C\, M^{-k} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 |F|_\rho \big(1 + (\alpha M)^3\big) \\ &= C\, M^{-k} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \frac{K(0,\rho)}{M} \big(1 + (\alpha M)^3\big). \qquad \text{(C.13)}\end{aligned}$$

For $j > k/2$, we have that $j - 1 > 6$ (still, since $k > 14$) and by (3.1)

$$\begin{aligned}\|\chi R(z,H_W)^j \chi_1 F Y^2 \chi_2 R(z,H_V)^{k-j+1}\|_1 \\ &\le \|\chi R(z,H_W)^j \chi_1 F Y\|_1 \|Y \chi_2 R(z,H_V)^{k-j+1}\|,\end{aligned}$$

and using the same procedure as above (now with Lemma B.12 on the first factor, since $j - 1 > 6$) we get, that the last term in (C.12) is bounded by the expression in (C.13) for all $j = 1, \dots, k$.

As for the first term in (C.12):

$$\begin{aligned}&\chi R(z,H_W)^j [\sqrt{\alpha^{-1}p^2 + \alpha^{-2}}, \chi_1] R(z,H_V)^{k-j+1} \\ &= \chi R(z,H_W)^j \left[\frac{1}{\pi}\int_0^\infty R_t C_1 R_t \sqrt{t}\, dt\right] R(z,H_V)^{k-j+1}\end{aligned}$$

with $C_1 = [\alpha^{-1}p^2, \chi_1]$. By a computation similar to that for the term

$$\chi R(z,H_W)^j \left[\frac{1}{\pi}\int_0^\infty R_t C_1 R_t \sqrt{t}\, dt\right] R(z,A)^{k-j+1}$$

in the proof of Lemma B.14 (see (B.64), (B.65), and (B.68)), we get that (for all $K > 3$ and $P \ge 1$)

$$\begin{aligned}&\|\chi R(z,H_W)^j [\sqrt{\alpha^{-1}p^2 + \alpha^{-2}}, \chi_1] R(z,H_V)^{k-j+1}\|_1 \\ &\le C \left(1 + \frac{1}{\sqrt{\alpha}}\frac{1}{d_M(z)}\right) \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \left(\frac{\beta}{\rho}\right)^{2K} \\ &\qquad \times \left\{ \left(\frac{(\,|z| + M\,)^{1/2}}{d_M(z)}\right)^{2K} + \frac{\alpha^P}{d_M(z)} \right\} \frac{1}{|\operatorname{Im}(z)|^k} \\ &\le C\, M^{-k} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \left(\frac{\beta}{\rho}\right)^{2K} \left(1 + \frac{1}{\sqrt{\alpha}}\frac{1}{M}\right) \left(\frac{1}{M^K} + \frac{\alpha^P}{M}\right)\end{aligned}$$

This is due to the fact that both

$$\|R(z,A)\| \le |\operatorname{Im}(z)|^{-1} \quad \text{and} \quad \|R(z,H_V)\| \le |\operatorname{Im}(z)|^{-1}.$$

This means, that

$$\begin{aligned} &\|\chi[R(\pm iM,H_V)^k - R(\pm iM,H_W)^k]\|_1 \\ &\le C\,M^{-k}\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \left\{ \left(\frac{\beta}{\rho}\right)^{2K}\left(\frac{1}{M^K}+\frac{\alpha^P}{M}\right)\left(1+\frac{1}{\sqrt{\alpha}}\frac{1}{M}\right) \right. \\ &\qquad\qquad \left. + \frac{K(0,\rho)}{M}\big(1+(\alpha M)^3\big) \right\} \end{aligned}$$

which proves the bound (C.10).

As for the bound (C.9), we have from (C.11) (with $k=1$) and (C.5) in Lemma C.2, that

$$\begin{aligned} &\|\chi[R(z,H_V)-R(z,H_W)]\| \\ &\qquad \le \|\chi[\chi_1 R(z,H_V) - R(z,H_W)\chi_1]\| + \|\chi R(z,H_W)\phi\| \\ &\qquad \le \|\chi R(z,H_W)[\sqrt{\alpha^{-1}p^2+\alpha^{-2}},\chi_1]R(z,H_V)\| \\ &\qquad\quad + \|\chi R(z,H_W)\phi\| + \|\chi R(z,H_W)\chi_1 F Y^2 R(z,H_V)\|. \end{aligned}$$

By using the estimate (B.9) from Lemma B.2, we get, for any $N \ge 1$ and $P \ge 1$, that

$$\|\chi R(z,H_W)\phi\| \le C\,\frac{1}{d_M(z)}\left(\frac{\beta}{\rho}\right)^N \left\{ \left(\frac{(\,|z|+M\,)^{1/2}}{d_M(z)}\right)^N + \frac{\alpha^P}{d_M(z)} \right\}$$

whereas using Lemma B.6 twice (with $\chi_1\chi_2 = \chi_1$ as before)

$$\begin{aligned} &\|\chi R(z,H_W)\chi_1 F Y^2 R(z,H_V)\| \\ &\qquad \le \|\chi R(z,H_W)\chi_1 Y\|\,|F|_\rho\,\|\chi_2 Y R(z,H_V)\| \\ &\qquad \le C\,\frac{(\,|z|+M\,)^{1/2}}{d_M(z)}\,|F|_\rho\,\frac{(\,|z|+M\,)^{1/2}}{d_M(z)} \\ &\qquad = C\,\frac{1}{d_M(z)^2}\cdot(\,|z|+M\,)|F|_\rho. \end{aligned}$$

A computation like the one in the proof of Lemma B.14 (see (B.63), (B.64), (B.65) and (B.68)) shows that (for any $N \ge 1$ and $P \ge 1$)

$$\begin{aligned} &\|\chi R(z,H_W)[\sqrt{\alpha^{-1}p^2+\alpha^{-2}},\chi_1]R(z,H_V)\| \\ &\le \frac{C}{d_M(z)}\left(1+\frac{1}{\sqrt{\alpha}}\frac{1}{d_M(z)}\right)\left(\frac{\beta}{\rho}\right)^N \left\{ \left(\frac{(\,|z|+M\,)^{1/2}}{d_M(z)}\right)^N + \frac{\alpha^P}{d_M(z)} \right\}, \end{aligned}$$

the essential difference being the same as that that accounts for the factor $\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3$ lacking in the estimate (B.9), compared to (B.7) (see the proof of Lemma B.2), namely the use of Lemma B.4 in the latter. Also, we use that we have $\|R(z, H_V)\| \le (d_M(z))^{-1}$, whereas in Lemma B.14 we used $\|R(z, A)\| \le |\operatorname{Im}(z)|^{-1}$. This means that

$$\begin{aligned}
&\Big\|\chi\big[R(z,H_V) - R(z,H_W)\big]\Big\| \\
&\quad \le \frac{C}{d_M(z)}\left(1 + \frac{1}{\sqrt{\alpha}}\frac{1}{d_M(z)}\right)\left(\frac{\beta}{\rho}\right)^N \\
&\qquad \times \left\{\left(\frac{(\,|z| + M\,)^{1/2}}{d_M(z)}\right)^N + \frac{\alpha^P}{d_M(z)}\right\} \quad + \quad \frac{K(z,\rho)}{d_M(z)^2}
\end{aligned}$$

This proves the bound (C.9), and thereby the lemma. □

We now continue, as when studying the passage from H_V to A, with a result on differences of functions on H_V and H_W. The assumptions are as for Lemma C.2, that is, the potentials V and W have the form (C.4), with the function Y satisfying (C.3). Also, $\rho \ge \rho_0$. We then have the following:

Theorem C.4. *Let $g \in C^\infty(\mathbb{R})$ satisfy $g(\lambda) = 0$ for $\lambda \ge \lambda_0$ and that for some $s \ge 0, L \ge L_0 > 0$ we have*

$$|\partial^n g(\lambda)| \le C_n L^n \langle\lambda\rangle^s \quad , \quad \forall n \in \mathbb{N} \tag{C.14}$$

(here, $\langle\lambda\rangle = (1 + |\lambda|^2)^{1/2}$). Let χ be any function such that $\operatorname{supp}\chi \subset B(\rho/2)$, $|\chi| \le 1$. *Then, for any $N \ge 1$:*

$$\begin{aligned}
&\|\chi[g(H_V) - g(H_W)]\| \\
&\qquad \le C\, L^{N+3} M^{s+1}\left[\frac{1}{\sqrt{\alpha}}\left(\frac{\beta\sqrt{M}}{\rho}\right)^N + K(0,\rho)\right]
\end{aligned} \tag{C.15}$$

with $K(0,\rho) = M\,|F|_\rho = M\,\sup_{|x|\le\rho}|F(x)|$. The constants C_N do not depend on V nor χ.

Proof. This will go very much as the proof of Theorem B.18. The idea is to use the representation (B.71), and estimate the resulting differences in resolvents by Lemma C.3.

More precisely, letting $\lambda \in \mathbb{R}$ and $0 < |\tau| \le 1$, denote (as in the proof of Theorem B.18)

$$\delta(\lambda,\tau) = R(\lambda + i\tau, H_V) - R(\lambda + i\tau, H_W).$$

Now using Lemma C.3 (and remembering, that $0 < |\tau| \le 1 \le M$, so $|z| + M \le |\lambda| + 2M$, and that $\alpha \le \alpha_0$), we have, for any $N \ge 1$ and any $P \ge 1$, that

$$\begin{aligned}
&\|\delta(\lambda,\tau)\| \\
&\quad \le C\,\frac{1}{|\tau|^2}\left[\frac{1}{\sqrt{\alpha}}\left(\frac{\beta}{\rho}\right)^N\left\{\left(\frac{(\,|\lambda| + 2M\,)^{1/2}}{|\tau|}\right)^N + \frac{\alpha^P}{|\tau|}\right\} + 2K(\lambda,\rho)\right] \\
&\qquad\qquad\qquad\qquad \text{for all } \lambda \in \mathbb{R}.
\end{aligned} \tag{C.16}$$

As in Theorem B.18, we have to modify the function g, since this not of compact support, in order to use the representation (B.71). The difference will be, that in this case, both the operators in question have the same lower bound, namely $-M$. Let therefore $\zeta \in C^\infty(\mathbb{R})$ be the function introduced in the proof of Theorem B.18: A monotone function such that $\zeta(t) = 0, t \leq -2$ and $\zeta(t) = 1, t \geq -3/2$. Define then $\tilde{g} \in C_0^\infty(\mathbb{R}^3)$ by $\tilde{g}(\lambda) = \zeta(\lambda/M)g(\lambda)$. Then, since $H_V, H_W \geq -M$ by (C.3), we have, by the spectral theorem, that $\tilde{g}(H_V) = g(H_V)$ and $\tilde{g}(H_W) = g(H_W)$. Because of (C.14) we have, that

$$|\partial^n \tilde{g}(\lambda)| \leq \tilde{C}_n L^n \langle\lambda\rangle^s \quad , \quad \forall n \in \mathbb{N}, \tag{C.17}$$

again, as in the proof of Theorem B.18, with constants $\tilde{C}_n$ depending on the C_j's, L_0, and the derivatives of ζ but not on M; here we used that $L \geq L_0$ and $M \geq 1$. Using now (B.71), we get that

$$\begin{aligned}
\tilde{g}(H_V) - \tilde{g}(H_W) &= I_1^{(n)} + I_2^{(n)} \qquad \forall n \in \mathbb{N}, \text{ with} \\
I_1^{(n)} &= \sum_{j=0}^{n-1} \frac{1}{\pi j!} \int_{\mathbb{R}} \partial^j \tilde{g}(\lambda) \operatorname{Im}\left[i^j \delta(\lambda, 1)\right] d\lambda \\
I_2^{(n)} &= \frac{1}{\pi(n-1)!} \int_0^1 \tau^{n-1}\, d\tau \int_{\mathbb{R}} \partial^n \tilde{g}(\lambda) \operatorname{Im}\left[i^n \delta(\lambda, \tau)\right] d\lambda
\end{aligned}$$

where the integration in λ in fact only takes places over the interval $[-2M, \lambda_0]$. Choose $n = N+3$, then, using the estimates (C.16) and (C.17), we have, that (remember, that $|\tau| = 1$ in this integral)

$$\begin{aligned}
&\|\chi I_1^{(n)}\| \\
&\leq C\, L^{N+2} M^s \int_{-2M}^{\lambda_0} \left[\frac{1}{\sqrt{\alpha}} \left(\frac{\beta}{\rho}\right)^N \left((|\lambda| + M)^{\frac{N}{2}} + \alpha^P\right) + K(\lambda, \rho)\right] d\lambda \\
&\qquad \leq C\, L^{N+3} M^{s+1} \left[\frac{1}{\sqrt{\alpha}} \left(\frac{\beta\sqrt{M}}{\rho}\right)^N + K(0, \rho)\right].
\end{aligned}$$

Here we used, that $|\lambda| \leq C(\lambda_0)M$ on the interval $[-2M, \lambda_0]$, and therefore $K(\lambda, \rho) \leq C\, K(0, \lambda)$; also, $L \geq L_0$ and $\alpha \leq \alpha_0$. Similarly,

$$\begin{aligned}
\|\chi I_2^{(n)}\| &\leq C\, L^{N+3} M^s \Big\{ \int_0^1 d\tau \int_{-2M}^{\lambda_0} \left[\frac{1}{\sqrt{\alpha}} \left(\frac{\beta}{\rho}\right)^N \left((|\lambda| + M)^{\frac{N}{2}}\right)\right] d\lambda \\
&\qquad + \int_0^1 \tau^N\, d\tau \int_{-2M}^{\lambda_0} \left[\frac{1}{\sqrt{\alpha}} \left(\frac{\beta}{\rho}\right)^N \frac{\alpha^P}{|\tau|} + K(\lambda, \rho)\right] d\lambda \Big\} \\
&\qquad\quad \leq C\, L^{N+3} M^{s+1} \left[\frac{1}{\sqrt{\alpha}} \left(\frac{\beta\sqrt{M}}{\rho}\right)^N + K(0, \rho)\right].
\end{aligned}$$

Together with the bound on $\chi I_1^{(n)}$, this proves the bound (C.15) and so the lemma. $\square$

This result will help us estimate the trace norm of the difference $g(H_V)-g(H_W)$. The idea is to pass the problem to one (in trace norm) on differences of powers of resolvents, and one (in operator norm) on the difference with some auxiliary function, $\tilde{g}$, instead of g; see also Lemma B.10 and Lemma B.16.

Theorem C.5. *Let the potentials V and W have the form (C.4), with the function Y satisfying (C.3). Let $g \in C^\infty(\mathbb{R})$ satisfy $g(\lambda) = 0$ for $\lambda \geq \lambda_0$ and that for some $s \geq 0, L \geq L_0 > 0$ we have*

$$|\partial^n g(\lambda)| \leq C_n L^n \langle\lambda\rangle^s \quad , \quad \forall n \in \mathbb{N} \tag{C.18}$$

(here, $\langle\lambda\rangle = (1+|\lambda|^2)^{1/2}$). Let χ be any function such that $\operatorname{supp}\chi \subset B(\rho/2)$, *$|\chi| \leq 1$. Then, for any $K \geq 3$*

$$\begin{aligned}\big\|\chi\big[g(H_V)-g(H_W)\big]\chi\big\|_1 \leq C_K\, L^{2K+3} M^{s+1} &\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \\ \times &\left\{\frac{1}{\sqrt{\alpha}}\left(\frac{\beta\sqrt{M}}{\rho}\right)^{2K} + K(0,\rho)\right\}\Big(1+\big(\alpha M\big)^3\Big).\end{aligned} \tag{C.19}$$

The constants C_K do not depend on V, W or χ.

Proof. As said, the idea is to define some auxiliary function: Denote

$$\tilde{g}(\lambda) = (\lambda - iM)^k g(\lambda) \quad , \quad k > 14.$$

Then, with $z = iM$,

$$\begin{aligned} g(H_V) - g(H_W) &= R(z,H_V)^k \tilde{g}(H_V) - R(z,H_W)^k \tilde{g}(H_W) \\ &= \big[R(z,H_V)^k - R(z,H_W)^k\big]\tilde{g}(H_V) \\ &\quad + R(z,H_W)^k\big[\tilde{g}(H_V)-\tilde{g}(H_W)\big], \end{aligned}$$

so that, by (3.1),

$$\begin{aligned}\big\|\chi\big[g(H_V)-g(H_W)\big]\chi\big\|_1 \leq \|\chi\big[R(z,H_V)^k - R(z,H_W)^k\big]\|_1\|\tilde{g}(H_V)\chi\| \\ + \|\chi R(z,H_W)^k\|_1\|\big[\tilde{g}(H_V)-\tilde{g}(H_W)\big]\chi\|.\end{aligned} \tag{C.20}$$

Note, that since $z = iM$ and $K(z,\lambda) = (\,|z| + M\,)|F|_\rho$, we have that $K(z,\rho) \leq 2K(0,\rho)$. Since $k > 14$, using (C.10) from Lemma C.3 we get, for all $K > 3$ and all $P \geq 1$ the estimate

$$\begin{aligned}
&\|\chi\big[R(z,H_V)^k - R(z,H_W)^k\big]\|_1 \\
&\leq C_K\, M^{-k} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \Bigg\{ \left(\frac{\beta}{\rho}\right)^{2K} \left(\frac{1}{M^K} + \frac{\alpha^P}{M}\right) \left(1 + \frac{1}{\sqrt{\alpha}}\frac{1}{M}\right) \\
&\qquad\qquad + \frac{K(0,\rho)}{M}\big(1 + (\alpha M)^3\big) \Bigg\}.
\end{aligned}$$

Now, by the spectral theorem,

$$\|\tilde{g}(H_V)\| \leq \|f\|_\infty$$

for

$$f(\lambda) = (\lambda - iM)^k g(\lambda)\ , \qquad \lambda \in [-M, \lambda_0]$$

since $H_V \geq -M$ and $g(\lambda) = 0$ for $\lambda \geq \lambda_0$. Since $|g(\lambda)| \leq C_n L^n \langle\lambda\rangle^s$ and $M \geq 1$, we have, that $\|f\|_\infty \leq C\, M^{s+k}$, and so the first term in (C.20) is bounded by

$$\begin{aligned}
&C\, M^s \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \Bigg\{ \left(\frac{\beta}{\rho}\right)^{2K} \left(\frac{1}{M^K} + \frac{\alpha^P}{M}\right) \left(1 + \frac{1}{\sqrt{\alpha}}\frac{1}{M}\right) \\
&\qquad\qquad + \frac{K(0,\rho)}{M}\big(1 + (\alpha M)^3\big) \Bigg\} \\
&\leq C\, L^{2K+3} M^{s+1} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \\
&\qquad \times \left\{ \frac{1}{\sqrt{\alpha}} \left(\frac{\beta\sqrt{M}}{\rho}\right)^{2K} + K(0,\rho) \right\} \big(1 + (\alpha M)^3\big) \qquad \text{(C.21)}
\end{aligned}$$

since $M \geq 1$, $L \geq L_0$, and $\alpha \leq \alpha_0$. Next, using Lemma B.9 (since $k > 14$), we get the estimate

$$\|\chi R(z,H_W)^k\|_1 \leq C\, M^{-k} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \Big(1 + (\alpha M)^3\Big). \qquad \text{(C.22)}$$

Now, remember, that $\tilde{g}(\lambda) = (\lambda - iM)^k g(\lambda)$ with the function g satisfying $|g(\lambda)| \leq C_n L^n \langle\lambda\rangle^s$. This means, that

$$|\tilde{g}(\lambda)| \leq C_n L^n \langle\lambda\rangle^{\tilde{s}} \quad , \quad \forall n \in \mathbb{N}$$

with $\tilde{s} = s + k$. In this way, using Theorem C.4 on the function $\tilde{g}$ (with $N = 2K$), the last factor in the last term in (C.20) gets bounded as follows:

$$\|\big[\tilde{g}(H_V) - \tilde{g}(H_W)\big]\chi\| \leq C\, L^{2K+3} M^{\tilde{s}+1} \left[\frac{1}{\sqrt{\alpha}} \left(\frac{\beta\sqrt{M}}{\rho}\right)^{2K} + K(0,\rho) \right]$$

and so, using (C.22), the last term in (C.20) gets bounded by (remember, that $\tilde{s} = s + k$)

$$C\,L^{2K+3}M^{s+1}\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3\left\{\frac{1}{\sqrt{\alpha}}\left(\frac{\beta\sqrt{M}}{\rho}\right)^{2K}+K(0,\rho)\right\}\Big(1+(\alpha M)^3\Big).$$

Together with the bound (C.21) this proves the theorem. $\square$

We now combine the results of Theorem B.18 and Theorem C.5 into a result relating $\mathrm{Tr}\{\psi\, g(A)\}$ and $\mathrm{Tr}\{\psi\, g(H_W)\}$ for the particular case of the functions g_s:

Theorem C.6. *Suppose the operator A satisfies Assumption B.1 with $D = B(4\rho)$, $\rho \geq \rho_0$, and a potential V, along with the potential W having the form (C.4), with the function Y satisfying (C.3). Assume furthermore, that the function χ satisfies* $\operatorname{supp}\chi \subset B(r/2)$, $|\chi| \leq 1$, *for some r such that $\rho \geq r \geq \rho_0$. Let for $s \in [0,1]$:*

$$g_s(\lambda) = \begin{cases} |\lambda|^s & \lambda < 0 \\ 0 & \lambda \geq 0 \end{cases} \tag{C.23}$$

and $L_0 \geq 2$ be some fixed number. Then, for any $L \geq L_0$ and $K > 3$ we have

$$\begin{aligned}\big\|\chi\big[g_s(A) - g_s(H_W)\big]\chi\big\|_1 &\leq C_{K,1}\,L^{2K+3}M^{s+1}\left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3\Big(1+(\alpha M)^3\Big)\\ &\qquad\times\left\{\frac{1}{\sqrt{\alpha}}\left(\frac{\beta\sqrt{M}}{\rho}\right)^{2K}+K(0,\rho)\right\}\\ &\quad + C_{K,2}\,L^{-s}\left(\frac{r}{\sqrt{\alpha}\beta}\right)^3\left(1+(\alpha M)^3+\frac{1}{\sqrt{\alpha}}\left(\frac{\beta}{r}\right)^{2K}\right).\end{aligned} \tag{C.24}$$

The constants $C_{K,1}$ and $C_{K,2}$ do not depend on the potentials V and W, nor on the the function χ.

Proof. The idea is to 'cut away' the singularity of g_s around zero (see (C.23)), at distance $\sim 1/L$, by splitting g_s in a sum of two functions, estimating the contributions from the two individually.

To this end, let $\zeta \in C_0^\infty(\mathbb{R})$, $|\zeta| \leq 1$, be a non-negative function such that

$$\zeta(\lambda) = \left\{\begin{array}{cc} 1 & |\lambda| \leq \frac{1}{2} \\ 0 & |\lambda| \geq 1 \end{array}\right. .$$

Denote

$$g^{(1)}(\lambda) = g_s(\lambda)\zeta(L\lambda)$$

and

$$g^{(2)}(\lambda) = g_s(\lambda)\big(1 - \zeta(L\lambda)\big)$$

so that $g_s = g^{(1)} + g^{(2)}$. It is clear, that $g^{(2)} \in C^\infty$, since $g^{(2)}(\lambda) = 0$ for $|\lambda| \leq 1/2L$. Also,

$$|\partial^n g^{(2)}(\lambda)| \leq C_n L^n \langle\lambda\rangle^s \qquad \forall n \in \mathbb{N}$$

(here, $\langle\lambda\rangle = (1 + |\lambda|^2)^{1/2}$) by the definition of g_s and since $L \geq L_0$ (we get at most a factor of L^n, in the case when all derivatives fall on $\zeta(L\lambda)$).

Since $\operatorname{supp}\chi \subset B(r/2) \subset B(\rho/2)$ (as $\rho \geq r$), the conditions of Theorems B.18 and C.5 are satisfied (with the function $g^{(2)}$), and these two theorems give us that

$$\begin{aligned}
\big\|\chi\big[g^{(2)}(A) - g^{(2)}(H_W)\big]\chi\big\|_1 \leq \big\|\chi\big[g^{(2)}(A) - g^{(2)}(H_V)\big]\chi\big\|_1& \\
+ \big\|\chi\big[g^{(2)}(H_V) - g^{(2)}(H_W)\big]\chi\big\|_1& \\
\leq C_K\, L^{2K+3} M^{s+1} \left(\frac{\rho}{\sqrt{\alpha}\beta}\right)^3 \Big(1 + \big(\alpha M\big)^3\Big)& \\
\times \left\{\frac{1}{\sqrt{\alpha}}\left(\frac{\beta\sqrt{M}}{\rho}\right)^{2K} + K(0,\rho)\right\}&
\end{aligned} \tag{C.25}$$

To treat the part with $g^{(1)}$, that is, around the singularity of g_s, note that, with $L \geq L_0 \geq 2$,

$$\zeta(L\lambda)\zeta(\lambda) = \zeta(L\lambda) \qquad \forall\lambda \in \mathbb{R},$$

and so, by the spectral theorem and (3.1), with $T = A, H_W$

$$\begin{aligned}
\|\chi g^{(1)}(T)\chi\|_1 &= \|\chi g_s(T)\zeta(LT)\chi\|_1 = \|\chi g_s(T)\zeta(LT)\zeta(T)\chi\|_1 \\
&\leq \|\chi g_s(A)\zeta(LT)\|\,\|\chi\zeta(T)\|_1
\end{aligned}$$

Since, by construction,

$$\|g_s(\lambda)\zeta(L\lambda)\|_\infty \leq C\, L^{-s},$$

Lemma B.10 and Lemma B.16 give us (since $\zeta \in C_0^\infty(\mathbb{R})$), that (remember, that $\operatorname{supp}\chi \subset B(r/2)$)

$$\begin{aligned}
\|\chi\big(g^{(1)}(A) - g^{(1)}(H_W)\big)\chi\|_1 &\leq C\, L^{-s}\Big(\|\chi\zeta(A)\|_1 + \|\chi\zeta(H_W))\|_1\Big) \\
&\leq C\, L^{-s}\left(\frac{r}{\sqrt{\alpha}\beta}\right)^3\left(1 + (\alpha M)^3 + \frac{1}{\sqrt{\alpha}}\left(\frac{\beta}{r}\right)^{2K}\right).
\end{aligned} \tag{C.26}$$

Note, that the constants in Lemma B.10 and Lemma B.16 depend on the length of the support of the involved function (here, ζ), which is why we assume a lower bound on L_0.

The bounds (C.25) and (C.26) now establish the bound of the theorem, since $g_s = g^{(1)} + g^{(2)}$. $\square$

Appendix D. An A Priori Estimate

In this appendix we prove results analogous to those in appendix B. The difference is that results in this appendix will be uniform in $\alpha \in]0, \alpha_0]$. The price is that we do not get as good a behaviour in β.

Throughout this appendix, χ and ϕ will denote functions satisfying the condition (B.6):

$$\begin{aligned} \operatorname{supp}\chi \subset B(\rho), &\qquad 0 \le |\chi| \le 1 \\ \operatorname{supp}\phi \subset \mathbb{R}^3 \setminus B(\nu\rho), &\qquad 0 \le |\phi| \le 1 \end{aligned}$$

for some $\rho \ge \rho_0$ and $\nu > 1$. Note that (as in appendix B) we do not assume anything on the regularity of either χ or ϕ.

We start with an analogue of Lemma B.2:

Lemma D.1. *There exist constants C_1 and C_2 such that for all $\lambda \ge C_1$:*

$$\|\chi R(z,H)\phi\|_1 \le C_2 \beta^{-3} \lambda^{-5/2} \big(1 + (\alpha\lambda)^{5/2}\big) g(\lambda, z)^7 \tag{D.1}$$

with

$$g(\lambda, z) = \max\Big\{ \frac{\lambda}{|z|}, \frac{\sqrt{(\operatorname{Re}(z)+\lambda)^2 + (\operatorname{Im}(z))^2}}{|\operatorname{Im}(z)|} \Big\}.$$

Proof. The theme of the proof will be the following: for four functions, $F_1 = F_1(p,\mu)$ and $F_2 = F_2(p,\mu)$ for $p \in \mathbb{R}^3$ and $\mu \in \mathbb{R}$, and ζ, $\xi \in C_0^\infty(\mathbb{R}^3)$, we have by using (3.2):

$$\|AB\|_1 \le \|A\|_2 \|B\|_2$$

and Lemma B.4:

$$\|f_1(x) f_2(-i\nabla)\|_2 \le (2\pi)^{-3/2} \|f_1\|_{L^2(\mathbb{R}^3)} \|f_2\|_{L^2(\mathbb{R}^3)}$$

and the Cauchy-Schwarz inequality:

$$\int g_1(\mu) g_2(\mu)\, d\mu \le \Big(\int g_1(\mu)^2\, d\mu\Big)^{1/2} \Big(\int g_2(\mu)^2\, d\mu\Big)^{1/2}$$

that:

$$\begin{aligned} &\int \|F_1(-i\beta\nabla,\mu)\zeta(x)\xi(x)F_2(-i\beta\nabla,\mu)\|_1\, d\mu \\ &\quad\le (2\pi\beta)^{-3} \int \|F_1(p,\mu)\|_{L^2(d^3p)} \|\zeta\|_{L^2(d^3x)} \|\xi\|_{L^2(d^3x)} \|F_2(p,\mu)\|_{L^2(d^3p)}\, d\mu \\ &\quad\le (2\pi\beta)^{-3} \|\zeta\|_{L^2} \|\xi\|_{L^2} \\ &\qquad\quad \times \Big(\int \|F_1(p,\mu)\|^2_{L^2(d^3p)}\, d\mu\Big)^{1/2} \Big(\int \|F_2(p,\mu)\|^2_{L^2(d^3p)}\, d\mu\Big)^{1/2}. \end{aligned} \tag{D.2}$$

Remark D.2. We shall use the inequality (D.2) numerous times, for various choices of the functions F_1 and F_2. When we do so, we will always bound the L^2-norm of the corresponding functions ζ and ξ by constants. We here note that the analysis that follows will indicate that we can in fact gain any power of λ (paying in powers of the function g) and any power of β. We shall due to time pressure not pursue this further — here, we will bound all gain of β's by a constant, due to the fact that $\beta \in]0, \beta_0]$.

We start by taking a function $\chi_1 \in C_o^\infty(\mathbb{R}^3)$ such that $\chi\chi_1 = \chi$ and $\chi_1\phi = 0$. Then, by (B.12),

$$\chi R(z,H)\phi = \chi R(z,H)\big[H_0, \chi_1\big] R(z,H)\phi.$$

The idea of the proof is to keep in mind the 'classical' case with kinetic energy p^2, and separate off the terms that will be purely relativistic. For instance, in the case of p^2 we have that $\big[p^2, \chi_1\big]\phi = 0$ as seen by (B.16) whereas we have from the above that

$$\begin{aligned}\chi R(z,H)\phi = \chi R(z,H)\big[H_0, \big[H_0, \chi_1\big]\big] R(z,H)\phi \\ + \chi R(z,H)^2\big[H_0, \chi_1\big]\phi.\end{aligned} \tag{D.3}$$

The last term will turn out to be bounded in trace norm, with a bound tending to zero as $\alpha \to 0$; think of this as refinding the 'classical' result mentioned above in the limit $\alpha \to 0$.

Repeating to commute the (multiple) commutator in the first term in (D.3) to the right, we arrive at

$$\begin{aligned}\chi R(z,H)\phi = \chi R(z,H)^n \underbrace{[H_0, [H_0, \dots, [H_0, \chi_1]\dots]]}_{n\times H_0} R(z,H)\phi \\ + \sum_{j=1}^{n-1} \chi R(z,H)^{j+1} \underbrace{[H_0, [H_0, \dots, [H_0, \chi_1]\dots]]}_{j\times H_0} \phi.\end{aligned} \tag{D.4}$$

To get rid of the potential V in $R(z,H)$, in order to get a function purely of p (to use (D.2)), we note the following:

Lemma D.3. *For all $m \geq 1$ there exist constants $C(V,m)$, $a(V,m)$ and $b(V,m)$ and operators A_m and B_m such that for all $\lambda \geq C(V,m)$:*

$$R(z,H)^m = A_m(H_0+\lambda)^{-m} = (H_0+\lambda)^{-m}B_m \tag{D.5}$$

with

$$\|A_m\| \leq a(V,m)g(\lambda,z)^m \quad , \quad \|B_m\| \leq b(V,m)g(\lambda,z)^m,$$

where

$$g(\lambda,z) = \max\Big\{\frac{\lambda}{|z|}, \frac{\sqrt{(\mathrm{Re}(z)+\lambda)^2 + (\mathrm{Im}(z))^2}}{|\mathrm{Im}(z)|}\Big\}.$$

Remark D.4. We note that $g(\lambda,z) \geq 1$.

Proof. We have, for λ to be specified, that

$$R(z,H)^m = (H-z)^{-m}(H+\lambda)^m(H+\lambda)^{-m}.$$

Since H is self adjoint, we have by the spectral theorem that

$$\|(H-z)^{-m}(H+\lambda)^m\| \le \sup_{x\ge 0}\left|\frac{x+\lambda}{x-z}\right|^m = g(\lambda,z)^m \tag{D.6}$$

with

$$g(\lambda,z) = \max\left\{\frac{\lambda}{|z|},\ \frac{\sqrt{(\mathrm{Re}(z)+\lambda)^2+(\mathrm{Im}(z))^2}}{|\,\mathrm{Im}(z)|}\right\}.$$

Next, note that

$$(H+\lambda)^m = \big((H_0+\lambda)+V\big)^m = \sum_{j+k+l=m}(H_0+\lambda)^j V^k (H_0+\lambda)^l$$

and so formally

$$\begin{aligned}(H+\lambda)^{-m} &= \Big(\sum_{j+k+l=m}(H_0+\lambda)^j V^k(H_0+\lambda)^l\Big)^{-1}\\ &= \Big((H_0+\lambda)^{-m}\sum_{j+k+l=m}(H_0+\lambda)^{j-m}V^k(H_0+\lambda)^l\Big)^{-1}\\ &= \Big(1+\sum_{\substack{j+k+l=m\\ j\ne m}}(H_0+\lambda)^{-k}(H_0+\lambda)^{-l}V^k(H_0+\lambda)^l\Big)^{-1}(H_0+\lambda)^{-m}\end{aligned} \tag{D.7}$$

Remark D.5. Note that there are $2^{m-1}-1$ terms in the sum. Also, for $k\ne 0$, $\|(H_0+\lambda)^{-k}\| \le 1/|\lambda|^k$.

We wish to study the operator

$$(H_0+\lambda)^{-l}V^k(H_0+\lambda)^l.$$

To this end, we write this in Fourier space: with

$$h_0(p) = \sqrt{\alpha^{-1}p^2+\alpha^{-2}} - \alpha^{-1},$$

we have that

$$\begin{aligned}\Big[(H_0+\lambda)^{-l}V^k(H_0+\lambda)^l\psi\Big]^{\widehat{}}(p) &= (h_0(p)+\lambda)^{-l}\Big(V^k(H_0+\lambda)^l\psi\Big)^{\widehat{}}(p)\\ &= (h_0(p)+\lambda)^{-l}\Big(\widehat{(V^k)} * (H_0+\lambda)^l\psi\Big)(p)\\ &= \int \widehat{(V^k)}(p-q)\Big(\frac{h_0(q)+\lambda)}{h_0(p)+\lambda)}\Big)^l\hat\psi(q)\,d^3q\end{aligned} \tag{D.8}$$

Note that

$$h_0(p) = \frac{\left(\sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1}\right)\left(\sqrt{\alpha^{-1}p^2 + \alpha^{-2}} + \alpha^{-1}\right)}{\left(\sqrt{\alpha^{-1}p^2 + \alpha^{-2}} + \alpha^{-1}\right)}$$

$$= \frac{p^2}{\sqrt{\alpha p^2 + 1} + 1} \leq p^2/2. \tag{D.9}$$

Now, for $|q| \geq 2|p|$:

$$\frac{h_0(q)}{1 + |p-q|^2} \leq \frac{q^2/2}{1 + q^2/4} \leq 2,$$

and so, for $\lambda \geq 1$ (and $|q| \geq 2|p|$):

$$h_0(q) \leq 2(1 + |p-q|^2) \leq 2(1 + |p-q|^2)(h_0(p) + \lambda)$$

$$\Rightarrow \quad h_0(q) + \lambda \leq 3(1 + |p-q|^2)(h_0(p) + \lambda). \tag{D.10}$$

On the other hand, for $|q| \leq 2|p|$, using (D.9):

$$\frac{h_0(q)}{h_0(p)} = \frac{\sqrt{\alpha^{-1}q^2 + \alpha^{-2}} - \alpha^{-1}}{\sqrt{\alpha^{-1}p^2 + \alpha^{-2}} - \alpha^{-1}} = \frac{|q|}{|p|}\ \frac{\sqrt{\alpha + 1/|p|^2} + 1/|p|}{\sqrt{\alpha + 1/|q|^2} + 1/|q|} \leq 4,$$

which means that for $\lambda \geq 1$ (and $|q| \leq 2|p|$):

$$h_0(q) + \lambda \leq 4(h_0(p) + \lambda) \leq 4(1 + |p-q|^2)(h_0(p) + \lambda).$$

Together with (D.10) this means that

$$(1 + |p-q|^2)^{-1}\frac{h_0(q) + \lambda}{h_0(p) + \lambda} \leq 4 \qquad \forall p, q \in \mathbb{R}^3\ ,\ \forall \lambda \geq 1.$$

That is, with $\langle x \rangle = (1 + x^2)^{1/2}$:

$$\langle p - q \rangle^{-2l}\Big(\frac{h_0(q) + \lambda}{h_0(p) + \lambda}\Big)^l \leq 4^l \qquad \forall p, q \in \mathbb{R}^3\ ,\ \forall \lambda \geq 1. \tag{D.11}$$

We now go back to (D.8). Let first

$$V_{k,l}(p) = \langle p \rangle^{2l}\ \widehat{(V^k)}(p).$$

Since $V \in C_0^\infty(\mathbb{R}^3)$, we have that $V_{k,l} \in L^1(\mathbb{R}^3_p)$, as the Fourier transform $\widehat{V^k}$ is a Schwartz - function. Then, using (D.8), (D.11) and the Hausdorff - Young inequality, we get that for all $\lambda \geq 1$:

$$\Big\|\Big[(H_0 + \lambda)^{-l}V^k(H_0 + \lambda)^l\psi\Big]^{\widehat{}}\Big\|^2_{L^2(\mathbb{R}^3_p)}$$

$$= \int\Big|\int\widehat{(V^k)}(p-q)\Big(\frac{h_0(q) + \lambda)}{h_0(p) + \lambda)}\Big)^l\hat{\psi}(q)\,d^3q\Big|^2 d^3p$$

$$\leq 8^l\int\Big(\int\Big|\langle p - q \rangle^{2l}\ \widehat{(V^k)}(p-q)\Big|\ \Big|\hat{\psi}(q)\Big|\,d^3q\Big)^2 d^3p$$

$$= 8^l\ \Big\|\ \big|V_{k,l}\big| * |\psi|\ \Big\|^2_{L^2(\mathbb{R}^3_p)} \leq 8^l\ \|V_{k,l}\|^2_{L^1(\mathbb{R}^3)} \cdot \|\hat{\psi}\|^2_{L^2(\mathbb{R}^3_p)}.$$

By Plancherel's theorem this means that for all $\lambda \geq 1$:

$$\|(H_0+\lambda)^{-l}V^k(H_0+\lambda)^l\| \leq \sqrt{8^l}\,\big\|V_{k,l}\big\|_{L^1(\mathbb{R}^3)} \tag{D.12}$$

We return to (D.7). By the estimate (D.12) and Remark D.5, there exists a constant $C = C(m,V) \geq 1$ such that for all $\lambda \geq C(m,V) \geq 1$:

$$\begin{aligned}
&\Bigg\| \sum_{\substack{j+k+l=m \\ j\neq m}} (H_0+\lambda)^{-k}(H_0+\lambda)^{-l}V^k(H_0+\lambda)^l \Bigg\| \\
&\qquad \leq \frac{1}{|\lambda|} \sum_{\substack{j+k+l=m \\ j\neq m}} \Big\|(H_0+\lambda)^{-l}V^k(H_0+\lambda)^l\Big\| \;<\; 1.
\end{aligned}$$

This justifies the manipulation (D.7) for $\lambda \geq C(m,V)$ and shows that there exist constants $a(V,m)$ such that

$$\forall\,\lambda \geq C(m,V): \quad (H+\lambda)^{-m} = \tilde{A}_m(H_0+\lambda)^{-m}\;,\; \|\tilde{A}_m\| \leq a(V,m).$$

Together with the estimate (D.6) this proves the first half of the lemma. The second half follows by an analogous proof. $\square$

We now return to the proof of Lemma D.1. We will use Lemma D.3 on all factors of $R(z,H)$ in all the terms of the decomposition in (D.4). By Remark D.4, this will give us a common factor of $g(\lambda,z)^{n+1}$, with

$$g(\lambda,z) = \max\left\{\frac{\lambda}{|z|},\; \frac{\sqrt{(\mathrm{Re}(z)+\lambda)^2+(\mathrm{Im}(z))^2}}{|\,\mathrm{Im}(z)|}\right\}.$$

for $\lambda \geq C_2$ for some C_2. Recall next the formula (B.13):

$$\big[H_0,\chi_1\big] = \frac{1}{\pi}\int_0^\infty (\alpha p^2+1+t)^{-1}\big[p^2,\chi_1\big](\alpha p^2+1+t)^{-1}\sqrt{t}\,dt.$$

Using this repeatedly, together with the formula (B.14):

$$\big[R(z,T),\psi\big] = -R(z,T)\big[T,\psi\big][R(z,T)$$

we get (omitting all factors of $1/\pi$ and signs from now on) that

$$\begin{aligned}
&\underbrace{[H_0,[H_0,\ldots,[H_0,\chi_1]\ldots]]}_{k\times H_0} \\
&= \int_0^\infty \cdots \int_0^\infty \Big[\prod_{j=1}^k (\alpha p^2+1+t_j)^{-1}\Big]\,\underbrace{\big[p^2,\big[\ldots\big[p^2,\chi_1\big]\ldots\big]\big]}_{k\times p^2} \\
&\qquad\qquad \times \Big[\prod_{j=1}^k (\alpha p^2+1+t_j)^{-1}\Big]\prod_{j=1}^k \sqrt{t_j}\,dt_j.
\end{aligned}$$

From now on we will omit the multiple integral sign and just write $\int_0^\infty$ meaning integration over $[0,\infty[$ in all variables t_j. Recall also, from

Lemma B.21, that with $p=-i\beta\nabla$:

$$\underbrace{[p^2,[p^2,[\dots[p^2,\chi]\dots]]]}_{N\times p^2}=\big(-i\beta\big)^N\sum_{\substack{|\eta|+|\gamma|=2N\\|\eta|\leq N}}a(\eta,\gamma)\,(\partial^\gamma\chi)\,p^\eta. \tag{D.13}$$

Note that by a proof analogous to that of Lemma B.21, a similar formula with all the p's to the left holds.

We are now ready to embark on estimating each term in (D.4) in trace norm, $\|\ \cdot\ \|_1$. We will let $n=6$.

Firstly, by the discussion above, what we need to estimate for the first term in (D.4):

$$S_1=\chi R(z,H)^6\underbrace{[H_0,[H_0,\dots,[H_0,\chi_1]\dots]]}_{6\times H_0}R(z,H)\phi$$

is the trace norm of operators of the form

$$Q_1=\int_0^\infty(H_0+\lambda)^{-6}\Big[\prod_{j=1}^k(\alpha p^2+1+t_j)^{-1}\Big]p^\gamma\partial^\eta\chi_1$$
$$\times\Big[\prod_{j=1}^6(\alpha p^2+1+t_j)^{-1}\Big](H_0+\lambda)^{-1}\prod_{j=1}^6\sqrt{t_j}\,dt_j \tag{D.14}$$

with $|\gamma|\leq 6$ and $|\gamma+\eta|=12$. Using the inequality from (D.2) with

$$F_1=(H_0+\lambda)^{-6}\Big[\prod_{j=1}^k(\alpha p^2+1+t_j)^{-1}\Big]p^\gamma,$$

$$F_2=\Big[\prod_{j=1}^6(\alpha p^2+1+t_j)^{-1}\Big](H_0+\lambda)^{-1}$$

and

$$d\mu=\prod_{j=1}^6\sqrt{t_j}\,dt_j$$

(and writing $\partial^\eta\chi_1$ as a product of two functions ζ and ξ) we get that

$$\|Q_1\|_1\leq C\,(2\pi\beta)^{-3}$$
$$\Big\{\int_0^\infty\int_{\mathbb{R}^3}d^3p\,(H_0+\lambda)^{-12}\Big[\prod_{j=1}^k(\alpha p^2+1+t_j)^{-2}\Big]p^{2|\gamma|}\prod_{j=1}^6\sqrt{t_j}\,dt_j\Big\}^{1/2}$$
$$\times\Big\{\int_0^\infty\int_{\mathbb{R}^3}d^3p\Big[\prod_{j=1}^6(\alpha p^2+1+t_j)^{-2}\Big](H_0+\lambda)^{-2}\prod_{j=1}^6\sqrt{t_j}\,dt_j\Big\}^{1/2}. \tag{D.15}$$

Let us estimate each of the factors above individually:

$$\begin{aligned}
&\int_0^\infty \int_{\mathbb{R}^3} d^3p\,(H_0+\lambda)^{-12}\Big[\prod_{j=1}^{6}(\alpha p^2+1+t_j)^{-2}\Big]p^{2|\gamma|}\prod_{j=1}^{6}\sqrt{t_j}\,dt_j\\
&= \int_{\mathbb{R}^3} d^3p\left[(H_0+\lambda)^{-12}p^{2|\gamma|}\int_0^\infty \Big[\prod_{j=1}^{6}(\alpha p^2+1+t_j)^{-2}\Big]\prod_{j=1}^{6}\sqrt{t_j}\,dt_j\right]\\
&= {c_0}^4\int_{\mathbb{R}^3} d^3p\left[(H_0+\lambda)^{-12}p^{2|\gamma|}(\alpha p^2+1)^{-3}\right]
\end{aligned}$$

with $c_0=\int_0^\infty(1+t)^{-2}\sqrt{t}\,dt$, by perfoming the t_j-integrations by the change of variables $t_j=(\alpha p^2+1)s_j$.

Now, by (B.29), with $c=\sqrt{2}-1$,

$$\sqrt{y^2+1}-1\geq\begin{cases} c\,y, & y\geq 1\\ c\,y^2, & y\in[0,1]\end{cases} \tag{D.16}$$

and so, for $\alpha p^2\leq 1$:

$$(H_0+\lambda)^{-1}=\frac{\alpha}{\sqrt{\alpha p^2+1}-1+\alpha\lambda}\leq\frac{\alpha}{c\alpha p^2+\alpha\lambda}=\frac{1}{cp^2+\lambda} \tag{D.17}$$

(think of the RHS as (the constant $1/c$ times) the 'classical' resolvent of p^2 at $-\lambda/c$), whereas for $\alpha p^2\geq 1$:

$$(H_0+\lambda)^{-1}=\frac{\alpha}{\sqrt{\alpha p^2+1}-1+\alpha\lambda}\leq\frac{\alpha}{c\sqrt{\alpha}p+\alpha\lambda}. \tag{D.18}$$

This means that

$$\begin{aligned}
&\int_{\alpha p^2\leq 1} d^3p\,(H_0+\lambda)^{-12}p^{2|\gamma|}(\alpha p^2+1)^{-3}\\
&\leq\int_{\alpha p^2\leq 1} d^3p\,\frac{p^{2|\gamma|}}{(cp^2+\lambda)^{12}}(\alpha p^2+1)^{-3}\leq C\int_{\mathbb{R}^3}\frac{d^3p}{(cp^2+\lambda)^6}=C\,\lambda^{-9/2},
\end{aligned}$$

since $|\gamma|\leq 6$, and that

$$\begin{aligned}
&\int_{\alpha p^2\geq 1} d^3p\,(H_0+\lambda)^{-12}p^{2|\gamma|}(\alpha p^2+1)^{-3}\\
&\qquad\leq\int_{\alpha p^2\geq 1} d^3p\,\frac{\alpha^{12-|\gamma|}(\alpha p^2)^{|\gamma|}}{(c\sqrt{\alpha}p+\alpha\lambda)^{12}}(\alpha p^2+1)^{-3}\leq C(\alpha_0)\alpha^{9/2}
\end{aligned}$$

since $|\gamma|\leq 6$ and $\alpha\in]0,\alpha_0]$. In this way the first factor in (D.15) is bounded by

$$C\left(\lambda^{-9/2}+\alpha^{9/2}\right)^{1/2}.$$

For the second factor we have that

$$\int_0^\infty \int_{\mathbb{R}^3} d^3p \left[\prod_{j=1}^{k} (\alpha p^2 + 1 + t_j)^{-2}\right] (H_0 + \lambda)^{-2} \prod_{j=1}^{6} \sqrt{t_j}\, dt_j$$
$$= \int_{\mathbb{R}^3} d^3p\, (H_0 + \lambda)^{-2} (\alpha p^2 + 1)^{-3}$$

by performing the t_j−integrals as before. Using (D.17) and (D.18) we have that

$$\int_{\alpha p^2 \leq 1} d^3p\, (H_0 + \lambda)^{-2} (\alpha p^2 + 1)^{-3}$$
$$\leq \int_{\alpha p^2 \leq 1} \frac{d^3p}{(cp^2 + \lambda)^2} (\alpha p^2 + 1)^{-3} \leq C\, \lambda^{-1/2}$$

and that

$$\int_{\alpha p^2 \geq 1} d^3p\, (H_0 + \lambda)^{-2} (\alpha p^2 + 1)^{-3}$$
$$\leq \int_{\alpha p^2 \geq 1} d^3p\, \frac{\alpha^2}{(c\sqrt{\alpha} p + \alpha\lambda)^2} (\alpha p^2 + 1)^{-3} \leq C' \sqrt{\alpha}.$$

This means that the last factor in (D.15) is bounded by

$$C \left(\lambda^{-1/2} + \alpha^{1/2}\right)^{1/2}$$

and so

$$\begin{aligned} \|Q_1\|_1 &\leq C\, \beta^{-3} \big(\lambda^{-9/2} + \alpha^{9/2}\big)^{1/2} \big(\lambda^{-1/2} + \alpha^{1/2}\big)^{1/2} \\ &\leq C\, \beta^{-3} \lambda^{-5/2} \big(1 + (\alpha\lambda)^{5/2}\big). \end{aligned} \tag{D.19}$$

Look now at the term

$$S_2 = \chi R(z, H)^6 \underbrace{[H_0, [H_0, \ldots, [H_0, \chi_1] \ldots]]}_{5 \times H_0} \phi.$$

In the 'classical' case, with kinetic energy p^2, this term would have been zero:

$$\chi R(z, p^2 + V)^6 \underbrace{[p^2, [p^2, [\ldots [p^2, \chi_1] \ldots]]]}_{5 \times p^2} \phi = 0.$$

By Lemma D.1 we need to estimate the trace norm of the operator

$$Q_2 = \int_0^\infty (H_0 + \lambda)^{-6} \left[\prod_{j=1}^{5} (\alpha p^2 + 1 + t_j)^{-1}\right] \underbrace{[p^2, [p^2, [\ldots [p^2, \chi_1] \ldots]]]}_{5 \times p^2}$$
$$\times \left[\prod_{j=1}^{5} (\alpha p^2 + 1 + t_j)^{-1}\right] \phi \prod_{j=1}^{6} \sqrt{t_j}\, dt_j.$$

The idea is that commuting the function ϕ to the left, through the product $\prod_{j=1}^{5}(\alpha p^2+1+t_j)^{-1}$, we gain powers of α, using the fact that

$$\underbrace{[p^2,[p^2,[\ldots[p^2,\chi_1]\ldots]]]}_{5\times p^2}\phi=0.$$

More precisely, with $T_j=(\alpha p^2+1+t_j)^{-1}$:

$$\begin{aligned}
&\underbrace{[p^2,[p^2,[\ldots[p^2,\chi_1]\ldots]]]}_{5\times p^2}\prod_{j=1}^{5}(\alpha p^2+1+t_j)^{-1}\phi\\
&=\big[\ldots\big]T_1T_2T_3T_4T_5\phi\\
&=\big[\ldots\big]\Big\{T_1T_2T_3T_4\big[T_5,\phi\big]+T_1T_2T_3\big[T_4,\phi\big]T_5+T_1T_2\big[T_3,\phi\big]T_4T_5\\
&\qquad\qquad+T_1\big[T_2,\phi\big]T_3T_4T_5+\big[T_1,\phi\big]T_2T_3T_4T_5\Big\}\\
&=\big[\ldots\big]\Big\{T_1T_2T_3T_4T_5\big[\alpha p^2,\phi\big]T_5+T_1T_2T_3T_4\big[\alpha p^2,\phi\big]T_4T_5\\
&\qquad\qquad+T_1T_2T_3\big[\alpha p^2,\phi\big]T_3T_4T_5+T_1T_2\big[\alpha p^2,\phi\big]T_2T_3T_4T_5\\
&\qquad\qquad\qquad+T_1\big[\alpha p^2,\phi\big]T_1T_2T_3T_4T_5\Big\}.
\end{aligned}$$

Now, also $\big[\ldots\big]\cdot\big[\alpha p^2,\phi\big]=0$ (see (B.16)) and so the above equals (with $[\,2\,]=\big[\alpha p^2,\big[\alpha p^2,\phi\big]\big]$):

$$\begin{aligned}
\big[\ldots\big]\Big\{&T_1T_2T_3T_4T_5[\,2\,]T_5^2+T_1T_2T_3T_4[\,2\,]T_4T_5^2+T_1T_2T_3[\,2\,]T_3T_4T_5^2\\
&+T_1T_2[\,2\,]T_2T_3T_4T_5^2+T_1[\,2\,]T_1T_2T_3T_4T_5^2+T_1T_2T_3T_4[\,2\,]T_4^2T_5\\
&+T_1T_2T_3[\,2\,]T_3T_4^2T_5+T_1T_2[\,2\,]T_2T_3T_4^2T_5+T_1[\,2\,]T_1T_2T_3T_4^2T_5\\
&+T_1T_2T_3[\,2\,]T_3^2T_4T_5+T_1T_2[\,2\,]T_2T_3^2T_4T_5+T_1[\,2\,]T_1T_2T_3^2T_4T_5\\
&+T_1T_2[\,2\,]T_2^2T_3T_4T_5+T_1[\,2\,]T_1T_2^2T_3T_4T_5+T_1[\,2\,]T_1^2T_2T_3T_4T_5\Big\}.
\end{aligned}\tag{D.20}$$

Using (D.13) we get that

$$\|T_1T_2T_3T_4[\,2\,]T_5^2\|\le C\,\alpha\prod_{j=1}^{5}(1+t_j)^{-1}.$$

and using (3.1) this gives us that

$$
\begin{aligned}
&\|(H_0+\lambda)^{-6}\Big[\prod_{j=1}^{5} T_j\Big]\,[\ldots]\,T_1T_2T_3T_4T_5[\,2\,]T_5^2\|_1 \\
&\le C\,\alpha\Big\|(H_0+\lambda)^{-6}\Big[\prod_{j=1}^{5} T_j\Big]\,[\ldots]\,T_5\Big\|_1 \prod_{j=1}^{5}(1+t_j)^{-1} \\
&= C\,\alpha\Big\|(H_0+\lambda)^{-6}\Big[\prod_{j=1}^{5} T_j\Big]\,[\ldots]\,T_5 \prod_{j=1}^{5}(1+t_j)^{-1}\Big\|_1.
\end{aligned}
$$

Here,

$$
\begin{gathered}
[\ldots] = \underbrace{[p^2,[p^2,[\ldots[p^2,\chi_1]\ldots]]]}_{5\times p^2} \\
[\,2\,] = \big[\alpha p^2, \big[\alpha p^2, \phi\big]\big]
\end{gathered}
$$

Recalling the formula (D.13), we need to estimate the trace norm of terms of the form

$$
R_2 = (H_0+\lambda)^{-6}\Big[\prod_{j=1}^{5} T_j\Big]\partial^{\eta}\chi_1 p^{\gamma} T_5 \prod_{j=1}^{5}(1+t_j)^{-1}
$$

with $|\gamma| \le 5$ and $|\eta+\gamma| = 10$. Letting

$$
\begin{aligned}
F_1 &= (H_0+\lambda)^{-6}\prod_{j=1}^{5}(\alpha p^2+1+t_j)^{-1}p^{\gamma}, \\
F_2 &= (\alpha p^2+1+t_5)^{-1}\prod_{j=1}^{5}(1+t_j)^{-1}, \\
d\mu &= \prod_{j=1}^{5}\sqrt{t_j}\,dt_j
\end{aligned}
$$

we therefore get, by (D.2), that

$$
\begin{aligned}
&\|R_2\|_1 \le C\,(2\pi\beta)^{-3}\alpha \\
&\times\Big\{\int_0^{\infty}\int_{\mathbb{R}^3} d^3p\,(H_0+\lambda)^{-12}\Big[\prod_{j=1}^{5} T_j\Big]p^{2|\gamma|}\prod_{j=1}^{5}\sqrt{t_j}\,dt_j\Big\}^{1/2} \\
&\times\Big\{\int_0^{\infty}\int_{\mathbb{R}^3} d^3p\,(\alpha p^2+1+t_5)^{-2}\prod_{j=1}^{5}(1+t_j)^{-2}\sqrt{t_j}\,dt_j\Big\}^{1/2}. \qquad \text{(D.21)}
\end{aligned}
$$

Now, for the second factor,

$$\alpha \left\{ \int_0^\infty \int_{\mathbb{R}^3} d^3p \, (\alpha p^2 + 1 + t_5)^{-2} \prod_{j=1}^{5} (1 + t_j)^{-2} \sqrt{t_j} \, dt_j \right\}^{1/2}$$

$$\leq \alpha \left\{ \int_{\mathbb{R}^3} d^3p \, (\alpha p^2 + 1)^{-2} \right\}^{1/2} \left\{ \int_0^\infty (1+t)^{-2} \sqrt{t} \, dt \right\}^{1/2} \leq C \, \alpha^{1/4}. \tag{D.22}$$

As previously, performing the t_j-integrals, the first factor in (D.21) becomes (remember that $T_j = (\alpha p^2 + 1 + t_j)^{-1}$)

$$\int_0^\infty \int_{\mathbb{R}^3} d^3p \, (H_0 + \lambda)^{-12} \Big[\prod_{j=1}^{5} T_j \Big] p^{2|\gamma|} \prod_{j=1}^{5} \sqrt{t_j} \, dt_j$$

$$= {c_0}^5 \int_{\mathbb{R}^3} d^3p \, (H_0 + \lambda)^{-12} p^{2|\gamma|} (\alpha p^2 + 1)^{-5/2}, \tag{D.23}$$

still with $c_0 = \int_0^\infty (1+t)^{-2} \sqrt{t} \, dt$. Using (D.17) and (D.18), we have (since $|\gamma| \leq 5$) that

$$\int_{\alpha p^2 \leq 1} d^3p \, (H_0 + \lambda)^{-12} p^{2|\gamma|} (\alpha p^2 + 1)^{-5/2}$$

$$\leq C \int_{\mathbb{R}^3} \frac{d^3p}{(cp^2 + \lambda)^6} = C' \lambda^{-9/2}$$

and

$$\int_{\alpha p^2 \geq 1} d^3p \, (H_0 + \lambda)^{-12} p^{2|\gamma|} (\alpha p^2 + 1)^{-5/2}$$

$$\leq \int_{\alpha p^2 \geq 1} d^3p \, \frac{p^{2|\gamma|}}{(\alpha^{-1}(c\sqrt{\alpha} p + \alpha\lambda))^{12}} (\alpha p^2 + 1)^{-5/2} \leq \tilde{C} \, \alpha^{11/2}.$$

In this way,

$$(D.23) \leq C \, \lambda^{9/2} \big(1 + (\alpha\lambda)^5\big)$$

and so, using (D.22) above,

$$\|R_2\|_1 \leq C \, \beta^{-3} \alpha^{1/4} \lambda^{-9/4} \big(1 + (\alpha\lambda)^5\big)^{1/2}$$

$$\leq \tilde{C} \, \beta^{-3} \lambda^{-5/2} \big(1 + (\alpha\lambda)^{5/2}\big).$$

The same estimate can be proved in a similar way for the other 12 terms in (D.20), and so

$$\|Q_2\|_1 \leq C \, \beta^{-3} \lambda^{-5/2} \big(1 + (\alpha\lambda)^{5/2}\big).$$

An analysis similar to the above for the terms (see (D.4))

$$\chi R(z, H)^{j+1} \underbrace{[H_0, [H_0, \ldots, [H_0, \chi_1] \ldots]]}_{j \times H_0} \phi \quad , \quad j = 2, 3, 4,$$

leads to the same estimate. We note that the difference is the number of resolvents in front. In order to compensate for a lower power of resolvents (and therefore of λ), we need to gain more α's and therefore commutate more times in the analysis analogous to (D.20).

Finally, look at the last term in (D.4):

$$\begin{aligned}&\chi R(z,H)^2\big[H_0,\chi_1\big]\phi\\&=\chi R(z,H)^2\int_0^\infty(\alpha p^2+1+t)^{-1}\big[p^2,\chi_1\big](\alpha p^2+1+t)^{-1}\phi\sqrt{t}\,dt.\end{aligned}$$

As mentioned, for the 'classical' case of the kinetic energy being p^2 we have:

$$\chi R(z,p^2+V)^2\big[p^2,\chi_1\big]\phi=0$$

— we wish to commute ϕ through the operator $(\alpha p^2+1+t)^{-1}$ above and use that $\big[p^2,\chi_1\big]\phi=0$. Doing this repeatedly, we have (using (B.14)) that

$$\begin{aligned}S_3&=\chi R(z,H)^2\big[H_0,\chi_1\big]\phi\\&=\chi R(z,H)^2\int(\alpha p^2+1+t)^{-1}\big[p^2,\chi_1\big](\alpha p^2+1+t)^{-1}\\&\qquad\underbrace{\big[\alpha p^2,\big[\ldots[\alpha p^2,\chi_1\big]\ldots\big]\big]}_{k\times\alpha p^2}(\alpha p^2+1+t)^{-k}\sqrt{t}\,dt.\end{aligned}$$

By Lemma D.3, we need to estimate the trace norm of the operator

$$\begin{aligned}Q_3=(H_0+\lambda)^{-2}&\int(\alpha p^2+1+t)^{-1}\big[p^2,\chi_1\big](\alpha p^2+1+t)^{-1}\\&\underbrace{\big[\alpha p^2,\big[\ldots[\alpha p^2,\chi_1\big]\ldots\big]\big]}_{k\times\alpha p^2}(\alpha p^2+1+t)^{-k}\sqrt{t}\,dt.\end{aligned}$$

Now, by (D.13),

$$\begin{aligned}&\|\underbrace{\big[\alpha p^2,\big[\ldots[\alpha p^2,\chi_1\big]\ldots\big]\big]}_{k\times\alpha p^2}(\alpha p^2+1+t)^{-k}\|\\&\leq\big(\sqrt{\alpha}\beta\big)^k\sum_{\substack{|\eta|+|\gamma|=2k\\|\gamma|\leq k}}|a(\eta,\gamma)|\,\|\partial^\eta\chi\|_\infty\|(\sqrt{\alpha}p)^{|\gamma|}(\alpha p^2+1+t)^{-k}\|\\&\leq C\,\big(\sqrt{\alpha}\beta\big)^k(1+t)^{-k/2}\end{aligned}$$

and so, using (D.2) with (see also (B.16))

$$\begin{aligned}F_1&=(H_0+\lambda)^{-2}(\alpha p^2+1+t)^{-1}p\,(1+t)^{-k/4},\\F_2&=(\alpha p^2+1+t)^{-1}(1+t)^{-k/4},\\d\mu&=\sqrt{t}\,dt\end{aligned}$$

we get that

$$
\begin{aligned}
&\|Q_3\|_1 \le C\,(2\pi\beta)^{-3}\big(\sqrt{\alpha}\big)^k \\
&\times \Big\{\int_0^\infty \int_{\mathbb{R}^3} d^3p\;(H_0+\lambda)^{-4}p^2\,(\alpha p^2+1+t)^{-2}p^2\,(1+t)^{-k/2}\sqrt{t}\,dt\Big\}^{1/2} \\
&\times \Big\{\int_0^\infty \int_{\mathbb{R}^3} d^3p\;(\alpha p^2+1+t)^{-2}(1+t)^{-k/2}\sqrt{t}\,dt\Big\}^{1/2}.
\end{aligned}
$$

Now,

$$
\begin{aligned}
&\int_0^\infty \int_{\mathbb{R}^3} d^3p\;(\alpha p^2+1+t)^{-2}(1+t)^{-k/2}\sqrt{t}\,dt \\
&\le \Big(\alpha^{-3/2}\int_{\mathbb{R}^3} d^3q\;(q^2+1)^{-2}\Big)\int_0^\infty (1+t)^{-k/2}\sqrt{t}\,dt \le C\,\alpha^{-3/2}
\end{aligned}
$$

and

$$
\begin{aligned}
&\int_0^\infty \int_{\mathbb{R}^3} d^3p\;(H_0+\lambda)^{-4}(\alpha p^2+1+t)^{-2}p^2(1+t)^{-k/2}\sqrt{t}\,dt \\
&\le \Big(\int_{\mathbb{R}^3} d^3p\;(H_0+\lambda)^{-4}(\alpha p^2+1)^{-2}p^2\Big)\int_0^\infty (1+t)^{-k/2}\sqrt{t}\,dt.
\end{aligned}
$$

As before,

$$
\int_{\alpha p^2\le 1} d^3p\;(H_0+\lambda)^{-4}(\alpha p^2+1+t)^{-2}p^2 \le C\int_0^\infty \frac{dp}{(cp^2+\lambda)^2} = \tilde{C}\,\lambda^{-3/2},
$$

and

$$
\begin{aligned}
&\int_{\alpha p^2\ge 1} d^3p\;(H_0+\lambda)^{-4}(\alpha p^2+1+t)^{-2}p^2 \\
&\qquad\qquad \le \alpha^4\int_{\alpha p^2\ge 1}\frac{p^4\,dp}{(c\sqrt{\alpha}p+\alpha\lambda)^4}(\alpha p^2+1)^2 \le C'\,\alpha^{5/2}
\end{aligned}
$$

This leads to the estimate

$$
\begin{aligned}
\|Q_3\|_1 &\le C\,\beta^{-3}\big(\sqrt{\alpha}\big)^k\big(\lambda^{-3/2}+\alpha^{3/2}\big)^{1/2}\alpha^{-3/4} \\
&\le C\,\beta^{-3}\lambda^{-5/2}\big(1+(\alpha\lambda)^{5/2}\big).
\end{aligned}
$$

In this way,

$$
\|\chi R(z,H)\phi\|_1 \le C\,\beta^{-3}\lambda^{-5/2}\big(1+(\alpha\lambda)^{5/2}\big)g(\lambda,z)^7
$$

with

$$
g(\lambda,z) = \max\Big\{\frac{\lambda}{|z|},\;\frac{\sqrt{(\mathrm{Re}(z)+\lambda)^2+(\mathrm{Im}(z))^2}}{|\,\mathrm{Im}(z)|}\Big\}.
$$

This finishes the proof of the lemma. □

Remark D.6. In fact this analysis takes us even further. Noting that the factor $\lambda^{-5/2}$ stems from the occurence of the highest power of resolvents in the decomposition (D.4), we see that commuting even further (i. e., taking $n > 6$), we can in fact prove the estimate (D.1) with any negative power of λ. We have chosen the power $-5/2$ in order to get integrability in the proof of Theorem D.12. Also, by the formula (B.16) we see that we by the procedure of the proof (taking more and more commutators) could gain any power of β; see Remark D.2.

We next note that we can prove a similar estimate for the operator $\chi R(z,H)\,p\phi$:

Lemma D.7. *With χ and ϕ as before we have*

$$\|\chi R(z,H)\,p\phi\|_1 \leq C\,\beta^{-3}\lambda^{-5/2}\big(1+(\alpha\lambda)^{5/2}\big)g(\lambda,z)^9 \tag{D.24}$$

with

$$g(\lambda,z)=\max\Big\{\frac{\lambda}{|z|}\,,\ \frac{\sqrt{(\mathrm{Re}(z)+\lambda)^2+(\mathrm{Im}(z))^2}}{|\,\mathrm{Im}(z)|}\Big\}.$$

Proof. Choosing the function χ_1 as in the proof of Lemma D.1, we note that, analogously to (D.4), we have the decomposition

$$\begin{aligned}\chi R(z,H)p\phi &= \chi R(z,H)^n\underbrace{[H_0,[H_0,\dots,[H_0,\chi_1]\dots]]}_{n\times H_0}R(z,H)p\phi\\ &\qquad+\sum_{j=1}^{n-1}\chi R(z,H)^{j+1}\underbrace{[H_0,[H_0,\dots,[H_0,\chi_1]\dots]]}_{j\times H_0}p\phi.\end{aligned} \tag{D.25}$$

To bound the terms of the last sum in (D.25), we refer to the proof of Lemma D.1: here, compared to that proof, we need to bound another power of p. Commuting once more like (D.20) will gain another power of α and a factor of $(\alpha p^2+1+t_j)^{-1}$ for some j. (Here we use that $p\phi = \phi p - i\beta\nabla\phi$). This is enough to bound the p uniformly in $\alpha\in\,]0,\alpha_0]$:

$$\|\alpha(\alpha p^2+1+t_j)^{-1}p\| \leq \frac{\sqrt{\alpha}}{2\sqrt{1+t_j}} \leq C.$$

As for the first term in (D.25), we first note that since $p\phi=\phi p - i\beta\nabla\phi$ we only need to look at the term

$$\chi R(z,H)^n\underbrace{[H_0,[H_0,\dots,[H_0,\chi_1]\dots]]}_{n\times H_0}R(z,H)\phi p,$$

since the term with $\dots R(z,H)\nabla\phi$ will be covered by Lemma D.1. From the proof of that lemma we also have that

$$\begin{aligned}&\underbrace{[H_0,[H_0,\dots,[H_0,\chi_1]\dots]]}_{n\times H_0}R(z,H)\phi p\\ &= \int_0^\infty\Big[\prod_{j=1}^n(\alpha p^2+1+t_j)^{-1}\Big]\underbrace{[p^2,[\dots[p^2,\chi_1]\dots]]}_{n\times p^2}\\ &\qquad\qquad\times\Big[\prod_{j=1}^n(\alpha p^2+1+t_j)^{-1}\Big]R(z,H)\phi p\prod_{j=1}^n\sqrt{t_j}\,dt_j.\end{aligned}$$

We note that since $\underbrace{\big[p^2, \big[\dots \big[p^2, \chi_1\big]\big]\big]}_{n \times p^2} \phi = 0$ we have (by (B.14)) that

$$\begin{aligned}
&\underbrace{\big[p^2, \big[\dots \big[p^2, \chi_1\big]\dots\big]\big]}_{n \times p^2} \Big[\prod_{j=1}^{n} (\alpha p^2 + 1 + t_j)^{-1}\Big] R(z,H)\phi p \\
&= \big[p^2, \dots\big] \Big[\prod_{j=1}^{n} T_j\Big] \phi R(z,H) p \\
&+ \big[p^2, \dots\big] \Big[\prod_{j=1}^{n} T_j\Big] R(z,H) \big[H_0, \phi\big] R(z,H) p \\
&+ \big[p^2, \dots\big] \Big[\prod_{j=1}^{n-1} T_j\Big] T_j \big[\alpha p^2, \phi\big] T_j R(z,H) p + \cdots \\
&+ \big[p^2, \dots\big] T_1 \big[\alpha p^2, \phi\big] T_1 \Big[\prod_{j=2}^{n} T_j\Big] R(z,H) p.
\end{aligned} \tag{D.26}$$

We show that the operator $R(z,H)p$ is bounded: By Lemma D.3 we have that $R(z,H)p = A_1(H_0 + \lambda)^{-1} p$ with $\|A_1\| \leq a(V) g(\lambda, z)$. Secondly, (D.17) gives us for $\alpha p^2 \leq 1$:

$$(H_0 + \lambda)^{-1} p \leq \frac{p}{cp^2 + \lambda} \leq \frac{1}{2\sqrt{c\lambda}} \leq C$$

where $c = \sqrt{2} - 1$, and (D.18) gives us for $\alpha p^2 \geq 1$:

$$(H_0 + \lambda)^{-1} p \leq \frac{\alpha p}{\sqrt{\alpha} p + \alpha \lambda} \leq \sqrt{\alpha} \leq \sqrt{\alpha_0}.$$

Look at (D.26) above. Since the operator $R(z,H)p$ by the above is bounded independently of α, the result of the lemma follows for all but the second of the terms in (D.26), by the same proof as that of Lemma D.1 (but with an extra factor of $g(\lambda, z)$ and for $\lambda \geq C_3$ with a possibly larger constant C_3). What we need for the second term is a bound on the operator norm of the operator $\big[H_0, \phi\big] R(z,H)p$. Then the proof of the bound (D.24) for this term will follow from an analysis like the one for (D.14).

Let us look at the operator $\big[H_0, \phi\big] R(z,H)p$:

$$\begin{aligned}
&\big[H_0, \phi\big] R(z,H)p = \big[H_0, \phi\big] p R(z,H) + \big[H_0, \phi\big]\ \big[R(z,H), p\big] \\
&= \big[H_0, \phi\big] p (H_0 + \lambda)^{-1} A_1 + \big[H_0, \phi\big] R(z,H) \big[V, p\big] R(z,H) \\
&= \big[H_0, \phi\big] p (H_0 + \lambda)^{-1} A_1 + \big[H_0, \phi\big] (H_0 + \lambda)^{-1} A_1 \big[V, p\big] R(z,H).
\end{aligned}$$

Note that $\big[V, p\big] = i\beta \nabla V$ and so both A_1 and $A_1 \big[V, p\big] R(z,H)$ are bounded independently of $\alpha \in]0, \alpha_0]$ (giving rise to one, resp. two extra powers of $g(\lambda, z)$). This leaves us with the task of bounding the operators $\big[H_0, \phi\big] p (H_0 + \lambda)^{-1}$ and $\big[H_0, \phi\big] (H_0 + \lambda)^{-1}$.

Firstly, by (B.16):

$$
\begin{aligned}
&\big[H_0, \phi\big] p(H_0+\lambda)^{-1} \\
&= \int_0^\infty (\alpha p^2+1+t)^{-1}\big[p^2,\phi\big](\alpha p^2+1+t)^{-1}\sqrt{t}\,dt\,p(H_0+\lambda)^{-1} \\
&= (-2i\beta)\int_0^\infty (\alpha p^2+1+t)^{-1}\nabla\phi\cdot p(\alpha p^2+1+t)^{-1}\sqrt{t}\,dt\,p(H_0+\lambda)^{-1} \\
&- \beta^2\int_0^\infty (\alpha p^2+1+t)^{-1}\Delta\phi(\alpha p^2+1+t)^{-1}\sqrt{t}\,dt\,p(H_0+\lambda)^{-1}.
\end{aligned}
$$

Secondly, commute $\nabla\phi$, resp. $\Delta\phi$, through the factor $(\alpha p^2+1+t)^{-1}$ to the left. Then the above equals

$$
\begin{aligned}
&- 2i\beta\nabla\phi\cdot\Big(\int_0^\infty (\alpha p^2+1+t)^{-2}\sqrt{t}\,dt\,p\Big)p\,(H_0+\lambda)^{-1} \\
&- 2i\beta\int_0^\infty (\alpha p^2+1+t)^{-1}\big[\alpha p^2,\nabla\phi\big]p\,(\alpha p^2+1+t)^{-2}\sqrt{t}\,dt\,(H_0+\lambda)^{-1} \\
&- \beta^2\Delta\phi\int_0^\infty (\alpha p^2+1+t)^{-2}\sqrt{t}\,dt\,p\,(H_0+\lambda)^{-1} \\
&- \beta^2\int_0^\infty (\alpha p^2+1+t)^{-1}\big[\alpha p^2,\Delta\phi\big]p\,(\alpha p^2+1+t)^{-2}\sqrt{t}\,dt\,(H_0+\lambda)^{-1} \\
&= \big(-2c_0 i\beta\nabla\phi\cdot(\alpha p^2+1)^{-1/2}p\big)\,p\,(H_0+\lambda)^{-1} \\
&- c_0\beta^2\Delta\phi(\alpha p^2+1)^{-1/2}p\,(H_0+\lambda)^{-1} \\
&- 2i\beta\int_0^\infty (\alpha p^2+1+t)^{-1}\big[\alpha p^2,\nabla\phi\big]p\,(\alpha p^2+1+t)^{-2}\sqrt{t}\,dt\,(H_0+\lambda)^{-1} \\
&- \beta^2\int_0^\infty (\alpha p^2+1+t)^{-1}\big[\alpha p^2,\Delta\phi\big]p\,(\alpha p^2+1+t)^{-2}\sqrt{t}\,dt\,(H_0+\lambda)^{-1}
\end{aligned}
\tag{D.27}
$$

by performing the $t-$integration (using the usual change of variables, $t=(\alpha p^2+1)s$; here, as before, $c_0=\int_0^\infty(1+t)^{-2}\sqrt{t}\,dt$). Now,

$$
(\alpha p^2+1)^{-1/2}p^2\,(H_0+\lambda)^{-1} = \frac{\alpha p^2}{(\alpha p^2+1)^{1/2}\big(\sqrt{\alpha p^2+1}-1+\alpha\lambda\big)}
$$

and so by (D.17), for $\alpha p^2\le 1$ (with $c=\sqrt{2}-1$):

$$
(\alpha p^2+1)^{-1/2}p^2\,(H_0+\lambda)^{-1} \le \frac{\alpha p^2}{(\alpha p^2+1)^{1/2}(c\alpha p^2+\alpha\lambda)} \le \frac{\alpha p^2}{c\alpha p^2} = \frac{1}{c}
$$

and by (D.18), for $\alpha p^2\ge 1$:

$$
\begin{aligned}
(\alpha p^2+1)^{-1/2}p^2\,(H_0+\lambda)^{-1} &\le \frac{\alpha p^2}{(\alpha p^2+1)^{1/2}(c\sqrt{\alpha}p+\alpha\lambda)} \\
&\le \frac{\alpha p^2}{\sqrt{\alpha p^2}c\sqrt{\alpha}p} = \frac{1}{c}.
\end{aligned}
$$

Then, by the spectral theorem:

$$\|(\alpha p^2+1)^{-1/2}p^2\,(H_0+\lambda)^{-1}\| \leq \frac{1}{c}.$$

Similarly:

$$(\alpha p^2+1)^{-1/2}p\,(H_0+\lambda)^{-1} = \sqrt{\alpha}\frac{\sqrt{\alpha}p}{(\alpha p^2+1)^{1/2}\big(\sqrt{\alpha p^2+1}-1+\alpha\lambda\big)}$$

and so, for $\alpha p^2 \leq 1$:

$$\begin{aligned}(\alpha p^2+1)^{-1/2}p\,(H_0+\lambda)^{-1} &\leq \frac{\alpha p}{(\alpha p^2+1)^{1/2}(c\alpha p^2+\alpha\lambda)}\\ &\leq \frac{p}{cp^2+\lambda} \leq \frac{1}{2\sqrt{c\lambda}} \leq C,\end{aligned}$$

and for $\alpha p^2 \geq 1$:

$$\begin{aligned}(\alpha p^2+1)^{-1/2}p\,(H_0+\lambda)^{-1} &\leq \sqrt{\alpha}\frac{\sqrt{\alpha}p}{(\alpha p^2+1)^{1/2}(c\sqrt{\alpha}p+\alpha\lambda)}\\ &\leq \sqrt{\alpha}/c \leq \sqrt{\alpha_0}/c.\end{aligned}$$

Using the spectral theorem this means that

$$\|(\alpha p^2+1)^{-1/2}p\,(H_0+\lambda)^{-1}\| \leq C.$$

This leaves us with the last two terms in (D.27). Now,

$$\frac{p}{(H_0+\lambda)} = \frac{\alpha p}{\sqrt{\alpha p^2+1}-1+\alpha\lambda}$$

and so by (D.17), for $\alpha p^2 \leq 1$ and $\lambda \geq 1$:

$$\frac{p}{(H_0+\lambda)} \leq \frac{\alpha p}{\alpha p^2+\alpha\lambda} \leq \frac{1}{2}$$

and by (D.18), for $\alpha p^2 \geq 1$:

$$\frac{p}{(H_0+\lambda)} \leq \frac{\alpha p}{\sqrt{\alpha}p+\alpha\lambda} \leq \sqrt{\alpha_0}.$$

By the above and the spectral theorem:

$$\|p(H_0+\lambda)^{-1}\| \leq C.$$

Using (B.16) we get that

$$\begin{aligned}&\|2i\beta\int_0^\infty(\alpha p^2+1+t)^{-1}\big[\alpha p^2,\nabla\phi\big](\alpha p^2+1+t)^{-2}\sqrt{t}\,dt\,p\,(H_0+\lambda)^{-1}\|\\ &\quad\leq C\,\beta^2\int_0^\infty\|(\alpha p^2+1+t)^{-1}\big(2\sqrt{\alpha}p\cdot\nabla(\nabla\phi)\\ &\qquad\qquad - i\sqrt{\alpha}\beta\Delta(\nabla\phi)\big)(\alpha p^2+1+t)^{-2}\|\sqrt{t}\,dt\\ &\quad\leq C\,\beta^2\int_0^\infty(1+t)^{-2}\sqrt{t}\,dt \leq C'.\end{aligned}$$

The proof for the other term is the same.

This finishes the proof of the lemma. □

Until now, we have only dealt with the operator H. We now embark on studying the 'abstract' operator A, assumed only to equal H in part of space; more specifically, we assume A to satisfy Assumption B.1 with $D = B(4\rho)$ for some $\rho \geq \rho_0$ with $\rho_0 > 0$ some fixed number.

We can now prove the analogue of Lemma B.14 (with $k = 1$):

Lemma D.8. *Suppose A satisfies Assumption B.1 with $D = B(4\rho)$, $\rho \geq \rho_0$, and that $\operatorname{supp}\chi \subset B(\rho)$, $|\chi| \leq 1$. Then there exists constants C_1 and C_2 such that for $\lambda \geq C_1$:*

$$\begin{aligned} &\|\chi\big(R(z,A) - R(z,H)\big)\|_1 \\ &\qquad \leq C_2\,\beta^{-3}\lambda^{-5/2}\big(1 + (\alpha\lambda)^{5/2}\big)\big(1 + \frac{1}{|\operatorname{Im}(z)|}\big) g(\lambda,z)^9 \end{aligned} \tag{D.28}$$

with

$$g(\lambda,z) = \max\Big\{\frac{\lambda}{|z|}\,,\ \frac{\sqrt{(\operatorname{Re}(z)+\lambda)^2 + (\operatorname{Im}(z))^2}}{|\operatorname{Im}(z)|}\Big\}.$$

Proof. This goes like the proof of Lemma B.14. Choosing a function $\chi_1 \in C_0^\infty(B(3\rho))$ such that $\chi\chi_1 = \chi$ we have, with $\phi_1 = 1 - \chi_1$, that

$$\chi\big(R(z,A) - R(z,H)\big) = \chi\big[\chi_1 R(z,A) - R(z,H)\chi_1\big] - \chi R(z,H)\phi_1.$$

The last term satisfies the bound (D.28) above due to Lemma D.1.

Using Lemma B.13, the first term equals

$$\chi R(z,H)\big[H_0,\chi_1\big]\bar{\zeta}_1 R(z,A) + \chi R(z,H)\ B\ R(z,A)$$

with an operator B satisfying

$$\|B\|_1 \leq C_N\left(\sqrt{\alpha}\beta\right)^N \quad \text{for all } N \in \mathbb{N}.$$

Here, $\zeta_1 \in C_0^\infty(D)$, such that $\zeta_1\chi_1 = \chi_1$. This means by Lemma D.3 that

$$\|\chi R(z,H)\ B\ R(z,A)\|_1 \leq C\,\lambda^{-1} g(\lambda,z)\,\frac{\left(\sqrt{\alpha}\beta\right)^N}{|\operatorname{Im} z|}$$

with $g(\lambda.z)$ as in the lemma.

We need a bound on the trace norm of the operator $\chi R(z,H)\big[H_0,\chi_1\big]$. The idea is, as before, that in the 'classical' case of kinetic energy p^2 (see (B.16)):

$$\begin{aligned} &\chi R(z,p^2+V)\big[p^2,\chi_1\big] \\ &\qquad = -i\beta\Big\{\chi R(z,p^2+V)\,p\nabla\chi_1 - i\beta\,\chi R(z,p^2+V)\Delta\chi_1\Big\} \end{aligned}$$

which would then both be covered by results like the ones in Lemma D.1 and Lemma D.7. We wish to bring us in a situation close to that:

$$
\begin{aligned}
&\chi R(z,H)\big[H_0,\chi_1\big] \\
&= \chi R(z,H)\int_0^\infty (\alpha p^2+1+t)^{-1}\big[p^2,\chi_1\big](\alpha p^2+1+t)^{-1}\sqrt{t}\,dt \\
&= \chi R(z,H)\big[p^2,\chi_1\big]\int_0^\infty (\alpha p^2+1+t)^{-2}\sqrt{t}\,dt \\
&+ \chi R(z,H)\int_0^\infty (\alpha p^2+1+t)^{-1}\big[\alpha p^2,\big[p^2,\chi_1\big]\big](\alpha p^2+1+t)^{-2}\sqrt{t}\,dt \\
&= \chi R(z,H)\big[p^2,\chi_1\big](\alpha p^2+1)^{-1/2} \\
&+ \alpha\chi R(z,H)\int_0^\infty (\alpha p^2+1+t)^{-1}\big[p^2,\big[p^2,\chi_1\big]\big](\alpha p^2+1+t)^{-2}\sqrt{t}\,dt.
\end{aligned}
$$

Here, the second equality follows from commuting $\big[p^2,\chi_1\big]$ through $(\alpha p^2+1+t)^{-1}$ to the left, and the last one follows from performing the $t-$integration, as seen earlier. Now, by (B.16)

$$\big[p^2,\chi_1\big] = -i\beta\big\{2p\cdot\nabla\chi_1 - i\beta\Delta\chi_1\big\}$$

and so the estimate (D.28) for the operator

$$\chi R(z,H)\big[p^2,\chi_1\big](\alpha p^2+1)^{-1/2}$$

follows from Lemma D.1 and Lemma D.7 (first using (3.1)). Now choose a second function $\chi_2 \in C_0^\infty(B(2\rho))$ such that $\chi_2\chi = \chi$ and $\chi_2\partial\chi_1 = 0$. Then, letting $\phi_2 = 1-\chi_2$:

$$
\begin{aligned}
&\alpha\chi R(z,H)\int_0^\infty (\alpha p^2+1+t)^{-1}\big[p^2,\big[p^2,\chi_1\big]\big](\alpha p^2+1+t)^{-2}\sqrt{t}\,dt \\
&= \alpha\chi R(z,H)\phi_2\int_0^\infty (\alpha p^2+1+t)^{-1}\big[p^2,\big[p^2,\chi_1\big]\big](\alpha p^2+1+t)^{-2}\sqrt{t}\,dt \\
&+ \alpha\chi R(z,H)\int_0^\infty \chi_2(\alpha p^2+1+t)^{-1}\big[p^2,\big[p^2,\chi_1\big]\big](\alpha p^2+1+t)^{-2}\sqrt{t}\,dt.
\end{aligned}
\tag{D.29}
$$

The functions χ and ϕ_2 now satisfy the conditions of Lemma D.1, and so

$$\|\chi R(z,H)\phi_2\|_1 \le C\beta^{-3}\lambda^{-5/2}\big(1+(\alpha\lambda)^{5/2}\big)g(\lambda,z)^7 \tag{D.30}$$

with

$$g(\lambda,z) = \max\Big\{\frac{\lambda}{|z|},\ \frac{\sqrt{(\mathrm{Re}(z)+\lambda)^2+(\mathrm{Im}(z))^2}}{|\,\mathrm{Im}(z)|}\Big\}.$$

Furthermore,

$$\Big\| \int_0^\infty (\alpha p^2+1+t)^{-1} p^2 (\alpha p^2+1+t)^{-2}\sqrt{t}\,dt \Big\|$$
$$\le \int_0^\infty \|p^2(\alpha p^2+1+t)^{-1}\|\;\|(\alpha p^2+1+t)^{-2}\|\sqrt{t}\,dt$$
$$\le \frac{C}{\alpha}\int_0^\infty (1+t)^{-2}\sqrt{t}\,dt.$$

Recalling the factor of α in (D.29) this and the estimate (D.30) above proves the bound (D.28) for the first term in (D.29) (remember the formula (D.13)).

As for the second term in (D.29):

$$\alpha\chi R(z,H)\int_0^\infty \chi_2(\alpha p^2+1+t)^{-1}\big[p^2,\big[p^2,\chi_1\big]\big](\alpha p^2+1+t)^{-2}\sqrt{t}\,dt$$

we use that $\chi_2\big[p^2,\big[p^2,\chi_1\big]\big]=0$ and commute $\big[p^2,\big[p^2,\chi_1\big]\big]$ to the left, through $(\alpha p^2+1+t)^{-1}$, to get

$$\alpha\int_0^\infty \chi R(z,H)\chi_2(\alpha p^2+1+t)^{-1}$$
$$\times\underbrace{\big[\alpha p^2,\dots,\big[p^2,\chi_2\big]\big]}_{n-2\times\alpha p^2,2\times p^2}(\alpha p^2+1+t)^{-n}\sqrt{t}\,dt.$$

We estimate $\chi R(z,H)$ and $\chi_2(\alpha p^2+1+t)^{-1}$ in norm, using Lemma D.3: for $\lambda\ge C(V)$ (for some suitable $C(V)$),

$$\|\chi R(z,H)\|\le C\,\lambda^{-1}g(\lambda,z)\quad,\quad \|\chi_2(\alpha p^2+1+t)^{-1}\|\le C\,(1+t)^{-1}$$

According to (D.13) we now need to estimate the trace norm of operators of the form (worst case)

$$Q=\big(\sqrt{\alpha}\big)^{n-2}\beta^n\int_0^\infty \partial^n\chi_1\big(\sqrt{\alpha}p\big)^n(\alpha p^2+1+t)^{-n}(1+t)^{-1}\sqrt{t}\,dt$$

Secondly, by Lemma B.22:

$$\|h_1(x)h_2(-i\beta\nabla)\|_1\le c_{\delta,\beta_0}\beta^{-\frac{3}{2}-\delta}\|h_1\|_\delta\|h_2\|_\delta$$

whenever

$$h_1,h_2\in L^2_\delta(\mathbb{R}^3)=\big\{f\;\big|\;\|f\|_\delta\equiv\|(1+x^2)^{\delta/2}f(x)\|_{L^2(\mathbb{R}^3)}<\infty\,\big\}$$

for some $\delta>3/2$. This means that

$$\|Q\|_1\le C\,\big(\sqrt{\alpha}\big)^{n-2}\beta^n\int_0^\infty \|\big(\sqrt{\alpha}p\big)^n(\alpha p^2+1+t)^{-n}\|_\delta(1+t)^{-1}\sqrt{t}\,dt \tag{D.31}$$

Now, by the Cauchy-Schwarz inequality:

$$\int_0^\infty \|\big(\sqrt{\alpha}p\big)^n(\alpha p^2+1+t)^{-n}\|_\delta(1+t)^{-1}\sqrt{t}\,dt$$
$$=\int_0^\infty \Big\{\int_{\mathbb{R}^3} d^3p\,(1+p^2)^{3+\epsilon}\big(\sqrt{\alpha}p\big)^{2n}(\alpha p^2+1+t)^{-2n}\Big\}^{1/2}(1+t)^{-1}\sqrt{t}\,dt$$
$$\leq \Big\{\int_0^\infty (1+t)^{-2}\sqrt{t}\,dt\Big\}^{1/2}$$
$$\times\Big\{\int_0^\infty\int_{\mathbb{R}^3} d^3p\,(1+p^2)^{3+\epsilon}\big(\sqrt{\alpha}p\big)^{2n}(\alpha p^2+1+t)^{-2n}\sqrt{t}\,dt\Big\}^{1/2}$$

Performing the $t-$integration in the last factor (by the usual change of variables $t=(\alpha p^2+1)s$), that factor equals

$$\Big\{C\int_{\mathbb{R}^3} d^3p\,(1+p^2)^{3+\epsilon}\big(\sqrt{\alpha}p\big)^{2n}(\alpha p^2+1)^{-2n+\frac{3}{2}}\Big\}^{1/2}$$
$$\leq\Big\{c_0\alpha^{-3/2}\int_{\mathbb{R}^3} d^3q\,(1+q^2/\alpha)^{3+\epsilon}q^{2n}(q^2+1)^{-2n+\frac{3}{2}}\Big\}^{1/2}$$
$$\leq C(\alpha_0)\,\alpha^{-9/4-\epsilon/2}$$

(by the change of variables $q=\sqrt{\alpha}p$) for some n sufficiently large, since for $q^2/\alpha\leq 1$ we have $1+q^2/\alpha\leq 2$ and for $q^2/\alpha\geq 1$, we have $1+q^2/\alpha\leq 2\alpha^{-1}q^2$ (remember that $\alpha\in\,]0,\alpha_0]$). Recalling the power of α in (D.31), this proves that the last term in (D.29) is bounded by

$$C_m\,\lambda^{-1}g(\lambda,z)\,\alpha^m$$

for any m. Since $g(\lambda,z)\geq 1$, this finishes the proof of the lemma. $\square$

We are now ready to embark on the main issue of this appendix, namely comparing $g(A)$ and $g(H)$ for various functions g. But first we prove two results on the trace norm of $\chi g(H)$:

Lemma D.9. *Let $\chi\in C_0^\infty(\mathbb{R}^3)$ and let $g\in C_0^\infty(\mathbb{R})$. Then*

$$\|\chi g(H)\|_1\leq C\,\beta^{-3}. \tag{D.32}$$

The constant is independent of $\alpha\in\,]0,\alpha_0]$.

Proof. By Lemma D.3 there exists, for all $k\in\mathbb{N}$, constants $C(V,k)$ and $a(V,k)$ and an operator B_k such that for $\lambda=C(V,k)$:

$$\chi g(H)=\chi(H_0+\lambda)^{-k}(H_0+\lambda)^kR(i\lambda,H)^k(H-i\lambda)^kg(H)$$
$$=\chi(H_0+\lambda)^{-k}B_k(H-i\lambda)^kg(H).$$

with $\|B_k\|\leq\tilde{C}(V,k)$. Firstly, by the spectral theorem:

$$\|(H-i\lambda)^kg(H)\|\leq C,$$

since $g\in C_0^\infty(\mathbb{R})$. Secondly, by Lemma B.22:

$$\|h_1(x)h_2(-i\beta\nabla)\|_1\leq c_{\delta,\beta_0}\beta^{-\frac{3}{2}-\delta}\|h_1\|_\delta\|h_2\|_\delta$$

whenever

$$h_1, h_2 \in L^2_\delta(\mathbb{R}^3) = \left\{ f \;\middle|\; \|f\|_\delta \equiv \|(1+x^2)^{\delta/2} f(x)\|_{L^2(\mathbb{R}^3)} < \infty \right\}$$

for some $\delta > 3/2$. Recall that

$$(H_0 + \lambda)^{-k} = f_k(-i\beta\nabla)$$

with

$$f_k(x) = \Big(\frac{\alpha}{\sqrt{\alpha x^2 + 1} - 1 + \alpha\lambda}\Big)^k \le \begin{cases} \left(\frac{1}{x^2+\lambda}\right)^k , & \sqrt{\alpha} x \le 1 \\ \left(\frac{\alpha}{\sqrt{\alpha} x + \alpha\lambda}\right)^k , & \sqrt{\alpha} x \ge 1 \end{cases}$$

and so it is obvious that $f_k \in L^2_\delta(\mathbb{R}^3)$ for k sufficiently large. This shows that for k large enough:

$$\|\chi(H_0 + \lambda)^{-k}\|_1 < \infty.$$

Now write $\psi = U\sqrt{|\chi|}\sqrt{|\chi|}$, $|U| = 1$. Then

$$\|\chi(H_0+\lambda)^{-2k}\|_1 = \|U\sqrt{|\chi|}(H_0+\lambda)^{-k}(H_0+\lambda)^{-k}\sqrt{|\chi|}\|_1$$

since $\|U\sqrt{|\chi|}(H_0+\lambda)^{-2k}\|_1 < \infty$ by the above and $\sqrt{|\chi|}$ is a bounded operator. We now use (3.2) and Lemma B.4:

$$\begin{aligned} &\|U\sqrt{|\chi|}(H_0+\lambda)^{-k}(H_0+\lambda)^{-k}\sqrt{|\chi|}\|_1 \\ &\qquad \le \|U\sqrt{|\chi|}(H_0+\lambda)^{-k}\|_2 \|\sqrt{|\chi|}(H_0+\lambda)^{-k}\|_2 \\ &\qquad \le (2\pi\beta)^{-3}\|U\sqrt{|\chi|}\|_{L^2(\mathbb{R}^3)}\|\sqrt{|\chi|}\|_{L^2(\mathbb{R}^3)}\|(H_0+\lambda)^{-k}\|^2_{L^2(\mathbb{R}^3)} \\ &\qquad = (2\pi\beta)^{-3}\|\chi\|_{L^1(\mathbb{R}^3)}\|(H_0+\lambda)^{-k}\|^2_{L^2(\mathbb{R}^3)}. \end{aligned}$$

Next, by (D.17):

$$\int_{\alpha p^2 \le 1} (H_0+\lambda)^{-2k}\, d^3p \le \int_{\alpha p^2 \le 1} \frac{d^3p}{(p^2+\lambda)^{2k}} \le \int_{\mathbb{R}^3} \frac{d^3p}{(p^2+\lambda)^{2k}} < \infty$$

for $k \ge 1$ and by (D.18):

$$\begin{aligned} \int_{\alpha p^2 \ge 1} (H_0+\lambda)^{-2k}\, d^3p &\le \int_{\alpha p^2 \ge 1} \frac{\alpha^{2k}\, d^3p}{(\sqrt{\alpha}p + \alpha\lambda)^{2k}} \\ &\le \alpha^{2k-3/2}\int_{q^2\ge 1}\frac{d^3q}{q^{2k}} \le C(\alpha_0) \end{aligned}$$

for all $\alpha \in]0, \alpha_0]$, when $k \ge 1$. This proves the bound (D.32). $\square$

Remark D.10. We note that in fact the lemma holds for $\chi \in L^1 \cap L^2_\delta(\mathbb{R}^3)$. We also note the splitting in two terms above, for which one (the first) is the one of the 'classical' kinetic energy p^2 and the other one goes to zero as $\alpha \to 0$, representing the relativistic part.

Secondly, we need the following lemma:

Lemma D.11. *For*

$$g_1(x) = \begin{cases} |x| \,, & x \le 0 \\ 0 \,, & x > 0 \end{cases}$$

and $\chi \in L^\infty(\mathbb{R}^3)$ *we have*

$$\|\chi g_1(H)\|_1 \le C\beta^{-3} \tag{D.33}$$

with a constant uniform in $\alpha \in]0, \alpha_0]$.

Proof. Firstly,

$$\|\chi g_1(H)\|_1 \le \|\chi\|_\infty \|g_1(H)\|_1.$$

Now, $\|g_1(H)\|_1 = S(H_0 + V)$, the sum of (the absolute values) of the negative eigenvalues of the operator $H = H_0 + V$. With

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

we have, by an inequality by Daubechies [2, see (2.1), (2.2) & (2.10)] (see also the proof of Lemma E.2), that

$$S(H_0 + V) \le k_3 \int_{\mathbb{R}^3} d^3x \left(\int_0^{W(x)} du \, [T^{-1}(u)]^3 \right)$$

with $W = \max\{0, -V\}$ and $k_3 = 1/(6\pi^2)$. Now,

$$T^{-1}(u) = \frac{\sqrt{2u}}{\beta} \sqrt{1 + \frac{\alpha u}{2}}$$

and so, making a Taylor expansion like in the proof of Lemma E.2, we get that

$$\begin{aligned} &S(H_0 + V) \\ &\quad \le \beta^{-3} k_3 \int_{\mathbb{R}^3} d^3x \, 2\sqrt{2} \left\{ \frac{2}{5} W(x)^{5/2} + \frac{3\alpha}{14} W(x)^{7/2} + \frac{\alpha^2}{48} W(x)^{9/2} \right\} \\ &\quad \le C(\alpha_0, V)\beta^{-3} \end{aligned}$$

since $V \in C_0^\infty(\mathbb{R}^3)$. This proves the lemma. ☐

Proving estimates on the trace norm of the difference $\chi\big(g(A) - g(H)\big)$ we will eventually be able to carry the estimates of Lemma D.9 and Lemma D.11 over to $\chi g(A)$ (for $g \in C_0^\infty(\mathbb{R})$, $g = g_1$ resp.)

We start with the following analogue of Theorem B.18:

Theorem D.12. *Suppose A satisfies Assumption B.1 with* $D = B(4\rho)$, $\rho \ge \rho_0$, *and that* $\operatorname{supp} \chi \subset B(\rho)$, $|\chi| \le 1$. *Let* $g \in C^\infty(\mathbb{R})$ *be a function such that* $g(\lambda) = 0$ *for* $\lambda \ge \lambda_0$ *and such that for some* $r \in [0, 1]$ *we have that*

$$|\partial^n g(\lambda)| \le C_n \langle\lambda\rangle^r \quad , \quad \forall n \in \mathbb{N} \tag{D.34}$$

(here, $\langle\lambda\rangle = (1 + |\lambda|^2)^{1/2}$*). Then*

$$\big\|\chi\big[g(A) - g(H)\big]\big\|_1 \le C\,\beta^{-3}, \tag{D.35}$$

with a constant C independent of $\alpha \in]0, \alpha_0]$.

Proof. As in the proof of Theorem B.18, we want to use the representation (B.71).

Let $\kappa \in \mathbb{R}$ and $0 < |\tau| \leq 1$. Denote

$$\delta(\kappa, \tau) = R(\kappa + i\tau, A) - R(\kappa + i\tau, H).$$

Then, according to (D.28), for $\lambda \geq C_1$ for some constant C_1:

$$\begin{aligned} &\|\chi\delta(\kappa,\tau)\|_1 \\ &\leq C\,\beta^{-3}\lambda^{-5/2}\big(1+(\alpha\lambda)^{5/2}\big)\tau^{-1}\max\Big\{\frac{\lambda}{\sqrt{\kappa^2+\tau^2}}, \frac{\sqrt{(\kappa+\lambda)^2+\tau^2}}{|\tau|}\Big\}^9. \end{aligned} \tag{D.36}$$

Here we used that $0 < |\tau| \leq 1$. For $\kappa \in [-C_1, \lambda_0]$, let $\lambda = C_1$, then (since $\alpha \in]0, \alpha_0]$):

$$\|\chi\delta(\kappa,\tau)\|_1 \leq C'\,\beta^{-3}\,\frac{1}{|\tau|^{10}} \quad , \quad \kappa \in [-C_1, \lambda_0]. \tag{D.37}$$

For $\kappa \leq -C_1$, let $\lambda = -\kappa$, then

$$\|\chi\delta(\kappa,\tau)\|_1 \leq \bar{C}\beta^{-3}|\kappa|^{-5/2}\big(1+(\alpha|\kappa|)^{5/2}\big)\frac{1}{|\tau|} \quad , \quad \kappa \leq -C_1. \tag{D.38}$$

Next we note, as in the proof of Theorem B.18, that the representation in Proposition B.17 does strictly speaking not apply to the function g, since this is not of compact support. We therefore modify the function g as in the proof of Theorem B.18: we get a function $\tilde{g} \in C_0^\infty(\mathbb{R})$, with $\tilde{g}(\kappa) = 0$ for $\kappa \leq -2\tilde{M} \equiv -2\max\{M, \alpha^{-1}\}$ and such that $\tilde{g}(A) = g(A)$ and $\tilde{g}(H) = g(H)$. (Recall that $H \geq -M$ and $A \geq -\alpha^{-1}$). Also,

$$|\partial^n \tilde{g}(\kappa)| \leq \tilde{C}_n \langle\kappa\rangle^r \quad , \quad \forall n \in \mathbb{N}. \tag{D.39}$$

Using (B.71), we get that

$$\tilde{g}(A) - \tilde{g}(H) = J_1^{(n)} + J_2^{(n)} \qquad \forall n \in \mathbb{N},$$

with

$$\begin{aligned} J_1^{(n)} &= \sum_{j=0}^{n-1} \frac{1}{\pi j!} \int_{\mathbb{R}} \partial^j \tilde{g}(\kappa)\, \mathrm{Im}\left[i^j \delta(\kappa, 1)\right] d\kappa \\ J_2^{(n)} &= \frac{1}{\pi(n-1)!} \int_0^1 \tau^{n-1}\, d\tau \int_{\mathbb{R}} \partial^n \tilde{g}(\kappa)\, \mathrm{Im}\left[i^n \delta(\kappa, \tau)\right] d\kappa \end{aligned}$$

where the integration in κ in fact only takes places over the interval $[-2\tilde{M}, \lambda_0]$.

Now, by the estimates (D.37) and (D.38) we have that

$$\|\chi J_1^{(n)}\|_1 \le C\,\beta^{-3}\Big\{ \int_{-2\tilde M}^{-C_1} |\kappa|^r |\kappa|^{-5/2}\big(1 + (\alpha|\kappa|)^{5/2}\big)\,d\kappa + \int_{-C_1}^{\lambda_0} 1\,d\kappa \Big\} \le C\,\beta^{-3}. \tag{D.40}$$

Here we used that $r + 1 - 5/2 \le -1/2$, $\tilde M = \max\{M, \alpha^{-1}\}$ and $\alpha \in\,]0, \alpha_0]$. (The important fact is to note, that the power of κ is sufficiently negative as to give a positive power of α when integrated to α^{-1}, which is the worst case).

Next, still by the estimates (D.37) and (D.38), we get:

$$\|\chi J_1^{(n)}\|_1 \le C\,\beta^{-3}\Big\{ \int_0^1 \tau^{n-2}\,d\tau \int_{-2\tilde M}^{-C_1} |\kappa|^r |\kappa|^{-5/2}\big(1 + (\alpha|\kappa|)^{5/2}\big)\,d\kappa + \int_0^1 \tau^{n-11}\,d\tau \int_{-C_1}^{\lambda_0} 1\,d\kappa \Big\} \tag{D.41}$$

Choosing $n \ge 11$ we get, as in (D.40), that

$$\|\chi J_1^{(n)}\|_1 \le C\,\beta^{-3}.$$

This proves the lemma. $\square$

Remark D.13. We note that we can get a better result than this: as noted in Remark D.6, we can get arbitrarily good (that is, negative) powers of λ in the estimate (D.1). More importantly, we can get arbitrarily high (positive) powers of β. In fact, we expect to be able to carry all of this analysis through, as to get all of the results of appendix B, without the loss of powers of α; due to time pressure, we will not do this here — the results of this appendix will be enough for our purposes.

Using this and Lemma D.9 we can prove:

Lemma D.14. *For any function χ with* $\operatorname{supp}\chi \subset B(\rho)$, $|\chi| \le 1$ *and any $g \in C_0^\infty(\mathbb{R})$ we have (with A as in Theorem D.12) that*

$$\|\chi g(A)\|_1 \le C\,\beta^{-3} \tag{D.42}$$

with a constant independent of $\alpha \in\,]0, \alpha_0]$.

Proof. It suffices to pass via $\chi g(H)$:

$$\|\chi g(A)\|_1 \le \|\chi\big[g(A) - g(H)\big]\|_1 + \|\chi g(H)\|_1.$$

The estimate now follows from Theorem D.12 for the first term and from Lemma D.9 and Remark D.10 for the second one. $\square$

This allows us to return to $\chi\big[g(A) - g(H)\big]$ and prove a bound like the one in Theorem D.12 for $g = g_1$:

Lemma D.15. *For any function* χ *with* $\operatorname{supp}\chi \subset B(\rho)$, $|\chi| \leq 1$ *and*

$$g_1(x) = \begin{cases} |x|\,, & x \leq 0 \\ 0\,, & x > 0 \end{cases}$$

we have, with A *as in Theorem D.12:*

$$\|\chi\big(g_1(A) - g(H)\big)\chi\|_1 \leq C\,\beta^{-3} \tag{D.43}$$

with a constant independent of $\alpha \in \,]0, \alpha_0]$.

Proof. The idea is like that of the proof of Theorem C.6: to cut away the singularity at 0 of the function g_1: choose $\zeta \in C_0^\infty(\mathbb{R})$, $|\zeta| \leq 1$, to be a non-negative function such that

$$\zeta(\lambda) = \begin{cases} 1 & |\lambda| \leq \frac{1}{2} \\ 0 & |\lambda| \geq 1. \end{cases}$$

Denote

$$g^{(1)}(\lambda) = g_1(\lambda)\zeta(2\lambda)$$

and

$$g^{(2)}(\lambda) = g_1(\lambda)\big(1 - \zeta(2\lambda)\big)$$

so that $g_1 = g^{(1)} + g^{(2)}$. It is clear that $g^{(2)} \in C^\infty$, since $g^{(2)}(\lambda) = 0$ for $|\lambda| \leq 1/4$. Also,

$$|\partial^n g^{(2)}(\lambda)| \leq C_n \langle\lambda\rangle^1 \qquad \forall n \in \mathbb{N}$$

(here, $\langle\lambda\rangle = (1 + |\lambda|^2)^{1/2}$) by the definition of g_1. To treat the part with $g^{(1)}$, that is, around the singularity of g_1, note that

$$\zeta(2\lambda)\zeta(\lambda) = \zeta(2\lambda) \qquad \forall \lambda \in \mathbb{R},$$

and so, by the spectral theorem and (3.1), with $T = A, H$

$$\begin{aligned} \|\chi g^{(1)}(T)\chi\|_1 = \|\chi g_1(T)\zeta(2T)\chi\|_1 &= \|\chi g_1(T)\zeta(2T)\zeta(T)\chi\|_1 \\ &\leq \|\chi g_1(A)\zeta(2T)\|\;\|\chi\zeta(T)\|_1 \end{aligned}$$

Since, by the spectral theorem,

$$\|g_1(T)\zeta(2T)\| \leq \|g_1(\lambda)\zeta(2\lambda)\|_\infty \leq C,$$

we get from Lemma D.9 and Lemma D.14 (since $\zeta \in C_0^\infty(\mathbb{R})$) that

$$\begin{aligned} \|\chi\big(g^{(1)}(A) - g^{(1)}(H)\big)\chi\|_1 &\leq C\left(\|\chi\zeta(A)\|_1 + \|\chi\zeta(H))\|_1\right) \\ &\leq C'\,\beta^{-3}. \end{aligned} \tag{D.44}$$

□

We are ready to finish the 'bootstrapping':

Theorem D.16. *Suppose A satisfies Assumption B.1 with $D = B(4\rho)$, $\rho \geq \rho_0$, and that* $\operatorname{supp}\chi \subset B(\rho) \subset \mathbb{R}^3$, $|\chi| \leq 1$. *Let*

$$g_1(x) = \begin{cases} |x|\,, & x \leq 0 \\ 0\,, & x > 0. \end{cases}$$

Then

$$\|\chi g_1(A)\|_1 \leq C\,\beta^{-3}. \tag{D.45}$$

The constant C is independent of $\alpha \in]0,\alpha_0]$.

Proof. As in the proof of Lemma D.14, it suffices to pass via $\chi g(H)$:

$$\|\chi g(A)\|_1 \leq \|\chi\big(g(A) - g(H)\big)\|_1 + \|\chi g(H)\|_1.$$

The estimate now follows from Lemma D.15 for the first term and from Lemma D.11 for the second one. □

We now turn to the integral

$$\frac{1}{(2\pi\beta)^3}\int \chi(x)\, g_1(a_\alpha(x,p))\, d^3x\, d^3p.$$

By Remark 5.6 we have (since $g_1(\lambda) = 0$ for $x \geq 0$) that

$$\left|\frac{1}{(2\pi\beta)^3}\int \chi(x)\, g_1(a_\alpha(x,p))\, d^3x\, d^3p\right| \leq C\,\beta^{-3}. \tag{D.46}$$

Combining Theorem D.16 and the bound (D.46) this proves the main result of this appendix:

Proposition D.17. *Suppose A satisfies Assumption B.1 with $D = B(4\rho)$, $\rho \geq \rho_0$, and that* $\operatorname{supp}\chi \subset B(\rho) \subset \mathbb{R}^3$, $|\chi| \leq 1$. *Let*

$$g_1(x) = \begin{cases} |x|\,, & x \leq 0 \\ 0\,, & x > 0. \end{cases}$$

Then

$$\operatorname{Tr}\{\chi\, g(A)\} = \frac{1}{(2\pi\beta)^3}\int \chi(x)\, g(a_\alpha(x,p))\, d^3x\, d^3p + \mathcal{O}(\beta^{-3}), \tag{D.47}$$

with a remainder uniform in $\alpha \in]0,\alpha_0]$.

Appendix E. Decay of energy of eigenfunctions

In this appendix, we will prove a result on the energy of the 'tail' of all the eigenfunctions corresponding to the negative eigenvalues of a Herbst-operator, with Coulomb potential 'pushed up'; more precisely:

Lemma E.1. *Let*

$$H = H_0 + V = \sqrt{-\Delta + 1} - 1 - \frac{\delta}{|x|}$$

for $\delta < \frac{2}{\pi}$ *and let* $H_\kappa = H + \kappa$ *for some* $\kappa \in]0,1]$. *Let* $\{e_j\}$ *be the negative eigenvalues of* H *below* $-\kappa$ *and* $\{\phi_j\}$ *corresponding normalised eigenfunctions:*

$$H\phi_j = e_j\phi_j \quad , \quad e_j < -\kappa. \tag{E.1}$$

Then $\{e_j + \kappa\}$ *are the negative eigenvalues of* H_κ *with eigenfunctions* $\{\phi_j\}$. *Finally, let* χ_r *be the characteristic function of the set* $\mathbb{R}^3 \setminus B(r)$, *with* $r = a\,\kappa^{-1}$ *for some* $a > 1 + \delta$. *Then, for some constant* C*:*

$$0 \geq \sum_{e_j < -\kappa} (e_j + \kappa)\big(\phi_j, \chi_r\phi_j\big) \geq -C\,\sqrt{\kappa}. \tag{E.2}$$

Proof. Start by noting that

$$\sum_{e_j < -\kappa} (e_j + \kappa)\big(\phi_j, \chi_r\phi_j\big) \geq \sum_{e_j < -\kappa} e_j\big(\phi_j, \chi_r\phi_j\big) \tag{E.3}$$

since κ is positive. Next, choose a smooth version of the characteristic function χ_r: Let $\tilde{\chi}_r \in \mathcal{B}^\infty(\mathbb{R}^3)$, $|\tilde{\chi}_r| \leq 1$, be a function, monotone in $|x|$, such that $\tilde{\chi}_r(x) = 1$ for $|x| \geq r = a\,\kappa^{-1}$ and $\tilde{\chi}_r(x) = 0$ for $|x| \leq (a-1)\,\kappa^{-1}$, and such that $|\partial_l\tilde{\chi}_r| \leq c_1\kappa$ for $l = 1,2,3$, and $|\partial_k\partial_l\tilde{\chi}_r| \leq c_2\kappa^2$ for $k,l = 1,2,3$. Next, we decompose the sum on the RHS of (E.3) to take advantage of the fact that the potential $V = -\frac{\delta}{|x|}$ is not too negative for $|x| \geq (a-1)\kappa^{-1}$, first putting in the function $\tilde{\chi}_r$, using that $e_j\chi_r \geq e_j\tilde{\chi}_r^2$ (the eigenvalues are negative):

$$\begin{aligned}
0 &\geq \sum_{e_j<-\kappa} e_j\big(\phi_j, \chi_r\phi_j\big) \geq \sum_{e_j<-\kappa} e_j\big(\phi_j, \tilde{\chi}_r^2\phi_j\big) = \sum_{e_j<-\kappa} \big(\phi_j, \tilde{\chi}_r^2 H\phi_j\big) \\
&= \sum_{e_j<-\kappa} \big(\phi_j, \tilde{\chi}_r H\tilde{\chi}_r\phi_j\big) + \sum_{e_j<-\kappa} \big(\phi_j, \tilde{\chi}_r[\tilde{\chi}_r, H]\phi_j\big) \\
&\geq -\frac{\delta\kappa}{a-1}\sum_{e_j<-\kappa} \big(\phi_j, \tilde{\chi}_r^2\phi_j\big) + \sum_{e_j<-\kappa} \big(\phi_j, \tilde{\chi}_r[\tilde{\chi}_r, H]\phi_j\big) \\
&\qquad\qquad + \sum_{e_j<-\kappa} \big(\phi_j, \tilde{\chi}_r H_0\tilde{\chi}_r\phi_j\big) \\
&\geq \frac{\delta}{a-1}\sum_{e_j<-\kappa} e_j\big(\phi_j, \tilde{\chi}_r^2\phi_j\big) + \sum_{e_j<-\kappa} \big(\phi_j, \tilde{\chi}_r[\tilde{\chi}_r, H]\phi_j\big) \\
&\qquad\qquad + \sum_{e_j<-\kappa} \big(\phi_j, \tilde{\chi}_r H_0\tilde{\chi}_r\phi_j\big).
\end{aligned}$$

The first equation because of (E.1), the third inequality because

$$\tilde{\chi}_r V\tilde{\chi}_r \geq -\frac{\delta\kappa}{a-1}\,\tilde{\chi}_r^2 \tag{E.4}$$

with the given choice of $r = a\,\kappa^{-1}$ and $\tilde{\chi}_r$, and the fourth, because we are summing over e_j's that are smaller than $-\kappa$. This means, that

$$\Big(1 - \frac{\delta}{a-1}\Big) \sum_{e_j<-\kappa} e_j\big(\phi_j, \tilde{\chi}_r^2\phi_j\big) \\ \geq \sum_{e_j<-\kappa} \big(\phi_j, \tilde{\chi}_r[\tilde{\chi}_r, H]\phi_j\big) + \sum_{e_j<-\kappa} \big(\phi_j, \tilde{\chi}_r H_0 \tilde{\chi}_r \phi_j\big). \tag{E.5}$$

We now need to investigate the term $\big(\phi_j, \tilde{\chi}_r[\tilde{\chi}_r, H]\phi_j\big)$. To this end, recall from (B.13) and (B.16) that (with $p = -i\nabla$)

$$[\sqrt{p^2+1}, \tilde{\chi}_r] \\ = -\frac{i}{\pi}\int_0^\infty (p^2+1+t)^{-1}\big(p\cdot\nabla\tilde{\chi}_r + \nabla\tilde{\chi}_r\cdot p\big)(p^2+1+t)^{-1}\sqrt{t}\,dt. \tag{E.6}$$

Now, by (B.14), we have that

$$\int_0^\infty (p^2+1+t)^{-1}\,p\cdot\nabla\tilde{\chi}_r(p^2+1+t)^{-1}\sqrt{t}\,dt \\ = \Big(\int_0^\infty (p^2+1+t)^{-2}\,p\,\sqrt{t}\,dt\Big)\cdot\nabla\tilde{\chi}_r \\ + \sum_{l=1}^{3}\int_0^\infty (p^2+1+t)^{-2}\,p_l\,[p^2, \partial_l\tilde{\chi}_r]\,(p^2+1+t)^{-1}\sqrt{t}\,dt. \tag{E.7}$$

Starting with the first term in (E.7) we have, by the change of variables $t = (p^2+1)s$, that

$$\int_0^\infty (p^2+1+t)^{-2}\,p\,\sqrt{t}\,dt = (p^2+1)^{-1/2}p\int_0^\infty (1+s)^{-2}\sqrt{s}\,ds.$$

By the Cauchy-Schwarz inequality we then get that

$$\big(\phi_j\tilde{\chi}_r, \frac{i}{\pi}\Big(\int_0^\infty (p^2+1+t)^{-2}\,p\,\sqrt{t}\,dt\Big)\cdot\nabla\tilde{\chi}_r\,\phi_j\big) \\ = C_0\sum_{l=1}^{3}\Big(\frac{p_l}{(p^2+1)^{1/2}}\tilde{\chi}_r\phi_j, i\,\partial_l\tilde{\chi}_r\phi_j\Big) \\ \geq -C_0\sum_{l=1}^{3}\Big(\Big(\frac{p_l}{\big(p^2+1\big)^{1/2}}\Big)^2\phi_j\tilde{\chi}_r, \phi_j\tilde{\chi}_r\Big)^{\frac{1}{2}}\big(\partial_l\tilde{\chi}_r\phi_j, \partial_l\tilde{\chi}_r\phi_j\big)^{\frac{1}{2}} \tag{E.8}$$

with $C_0 = \frac{1}{\pi}\int_0^\infty (1+s)^{-2}\sqrt{s}\,ds > 0$.

We note that using (B.29):

$$\sqrt{y^2+1} - 1 \geq \begin{cases} c_0\,y, & y \geq 1 \\ c_0\,y^2, & y \in [0,1] \end{cases}$$

with $c_0 = \sqrt{2} - 1$, we have that for $|p| \in [0, 1]$:

$$(\sqrt{2} - 1)\frac{p^2}{p^2 + 1} \le (\sqrt{2} - 1)p^2 \le \sqrt{p^2 + 1} - 1$$

and for $|p| \ge 1$:

$$(\sqrt{2} - 1)\frac{p^2}{p^2 + 1} \le (\sqrt{2} - 1) \le (\sqrt{2} - 1)|p| \le \sqrt{p^2 + 1} - 1$$

which gives the estimate

$$\frac{p^2}{p^2 + 1} \le \frac{1}{\sqrt{2} - 1}\big(\sqrt{p^2 + 1} - 1\big) \qquad \forall p. \tag{E.9}$$

In this way, using (E.8) and (E.9), we get that

$$\begin{aligned} &\big(\phi_j \tilde{\chi}_r, \frac{i}{\pi}\big(\int_0^\infty (p^2 + 1 + t)^{-2}\, p \sqrt{t}\, dt\big) \cdot \nabla \tilde{\chi}_r\, \phi_j\big) \\ &\quad \ge -\frac{C_0}{\sqrt{\sqrt{2} - 1}}\big(\phi_j, \tilde{\chi}_r H_0 \tilde{\chi}_r \phi_j\big)^{\frac{1}{2}} \sum_{l=1}^{3} \big(\partial_l \tilde{\chi}_r \phi_j, \partial_l \tilde{\chi}_r \phi_j\big)^{\frac{1}{2}}. \end{aligned}$$

As for the second term in (E.7), by (B.14):

$$\begin{aligned} &\sum_{l=1}^{3} (p^2 + 1 + t)^{-2}\, p_l\, [p^2, \partial_l \tilde{\chi}_r]\, (p^2 + 1 + t)^{-1} \\ &= -i \sum_{l=1}^{3} \sum_{k=1}^{3} (p^2 + 1 + t)^{-2}\, p_l \\ &\qquad\qquad \times \Big(p_k\, \partial_k \partial_l \tilde{\chi}_r + \partial_k \partial_l \tilde{\chi}_r\, p_k\Big)(p^2 + 1 + t)^{-1}. \end{aligned} \tag{E.10}$$

By the spectral theorem,

$$\begin{aligned} \|(p^2 + 1 + t)^{-2}\, p_l\, p_k\| &\le \frac{1}{1 + t}, \\ \|(p^2 + 1 + t)^{-2}\, p_l\| &\le \frac{1}{(1 + t)^{3/2}} \\ \|(p^2 + 1 + t)^{-1}\, p_l\| &\le \frac{1}{(1 + t)^{1/2}} \\ \|(p^2 + 1 + t)^{-1}\| &\le \frac{1}{1 + t} \end{aligned}$$

and, using this and (E.10), we get the estimate

$$\begin{aligned} &\Big\| -\frac{i}{\pi} \sum_{l=1}^{3} \int_0^\infty (p^2 + 1 + t)^{-2}\, p_l\, [p^2, \partial_l \tilde{\chi}_r]\, (p^2 + 1 + t)^{-1} \sqrt{t}\, dt \Big\| \\ &\qquad\qquad \le \sum_{l=1}^{3} \sum_{k=1}^{3} 2C_0 \|\partial_k \partial_l \tilde{\chi}_r\|_\infty \le 18 c_2\, C_0 \kappa^2 \end{aligned} \tag{E.11}$$

with C_0 as above, since $|\partial_k \partial_l \tilde{\chi}_r| \leq c_2 \kappa^2$ by construction. By the inequality $\big(\psi, A\phi\big) \geq -\|A\|\|\psi\|\|\phi\|$, we get, since the eigenfunctions are normalised and $\tilde{\chi}_r \leq 1$, that

$$\begin{aligned}
\Big(\phi_j \tilde{\chi}_r, \frac{i}{\pi} \sum_{l=1}^{3} \int_0^\infty (p^2+1+t)^{-2}\, p_l\, [p^2, \partial_l \tilde{\chi}_r]\, (p^2+1+t)^{-1} \sqrt{t}\, dt\ \phi_j\Big) \\
\geq -18 c_2 C_0 \kappa^2 \big(\tilde{\chi}_r \phi_j, \tilde{\chi}_r \phi_j\big)^{\frac{1}{2}} \big(\phi_j, \phi_j\big)^{\frac{1}{2}} \geq -18 c_2 C_0 \kappa^2.
\end{aligned}$$

For the other term in (E.6), commute $\nabla \tilde{\chi}_r$ to the other side and do as above. This gives us that

$$\begin{aligned}
\big(\phi_j, \tilde{\chi}_r [\tilde{\chi}_r, H] \phi_j\big) &\geq -36 c_2 C_0 \kappa^2 \\
&\quad - \frac{2C_0}{\sqrt{\sqrt{2}-1}} \big(\phi_j, \tilde{\chi}_r H_0 \tilde{\chi}_r \phi_j\big)^{\frac{1}{2}} \sum_{l=1}^{3} \big(\partial_l \tilde{\chi}_r \phi_j, \partial_l \tilde{\chi}_r \phi_j\big)^{\frac{1}{2}}.
\end{aligned}$$

Going back to (E.5) this means (using that the inequality $(X-Y)^2 \geq 0$ gives $X^2 - cXY \geq -c^2 Y^2/4$ and the facts, that $\chi_{r/2} \partial_l \tilde{\chi}_r = \partial_l \tilde{\chi}_r$ and $|\partial_l \tilde{\chi}_r| \leq c_1 \kappa$) that

$$\begin{aligned}
&\Big(1 - \frac{\delta}{a-1}\Big) \sum_{e_j < -\kappa} e_j \big(\phi_j, \tilde{\chi}_r^2 \phi_j\big) \\
&\quad \geq \sum_{e_j < -\kappa} \big(\phi_j, \tilde{\chi}_r H_0 \tilde{\chi}_r \phi_j\big) - C_1 \kappa^2 \Bigg(\sum_{e_j < -\kappa} 1\Bigg) \\
&\quad - C_2 \sum_{e_j < -\kappa} \sum_{l=1}^{3} \big(\phi_j, \tilde{\chi}_r H_0 \tilde{\chi}_r \phi_j\big)^{\frac{1}{2}} \big(\partial_l \tilde{\chi}_r \chi_{r/2} \phi_j, \partial_l \tilde{\chi}_r \chi_{r/2} \phi_j\big)^{\frac{1}{2}} \\
&\quad \geq -C_1 \kappa^2 \Bigg(\sum_{e_j < -\kappa} 1\Bigg) + \frac{9 c_1^2 {C_2}^2}{4} \kappa \sum_{e_j < -\kappa} e_j \big(\chi_{r/2} \phi_j, \chi_{r/2} \phi_j\big)
\end{aligned}$$

with

$$\begin{aligned}
C_1 &= 36 c_2 C_0 \\
C_2 &= \frac{C_0}{\sqrt{\sqrt{2}-1}}.
\end{aligned}$$

Here we again used, that we sum over e_j's that are smaller than $-\kappa$. Using again, that $e_j \chi_r \geq e_j \tilde{\chi}_r^2$ this finally leads us to the estimate

$$\sum_{e_j < -\kappa} e_j \big(\phi_j, \chi_r \phi_j\big) \geq C_3 \kappa \sum_{e_j < -\kappa} e_j \big(\phi_j, \chi_{r/2} \phi_j\big) - C_4 \kappa^2 \Bigg(\sum_{e_j < -\kappa} 1\Bigg)$$

with

$$C_3 = \frac{9c_1^2{C_0}^2(a-1)}{4(\sqrt{2}-1)(a-1-\delta)}$$
$$C_4 = \frac{36c_2C_0(a-1)}{a-1-\delta}.$$

Denoting

$$E(\kappa, r) = \sum_{e_j<-\kappa} e_j\big(\phi_j, \chi_r\phi_j\big)$$

this proves, that, as long as $r = a\,\kappa^{-1}$, with $a > 1+\delta$, we have that

$$|E(\kappa, r)| \leq C_3\kappa\,|E(\kappa, r/2)| + C_4\kappa^2\left(\sum_{e_j<-\kappa} 1\right). \tag{E.12}$$

Since

$$|E(\kappa, r/2)| \leq \sum_{e_j<-\kappa} |e_j|\big(\phi_j, \phi_j\big)$$

the lemma know follows from the estimate (E.12) and the following lemma (see also (E.3)). □

Lemma E.2. *There exist constants C_5 and C_6 such that, for all $\kappa \in$ $]0,1]$:*

$$\sum_{e_j<-\kappa} |e_j| = \sum_{e_j<-\kappa} |e_j|\big(\phi_j, \phi_j\big) \leq C_5\,\frac{1}{\sqrt{\kappa}},$$
$$\sum_{e_j<-\kappa} 1 \leq C_6\,\frac{1}{\kappa\sqrt{\kappa}}. \tag{E.13}$$

Proof. This is a consequence of a generalisation of the Lieb-Thirring inequality (see Lieb and Thirring [22]) and of the Cwikel-Lieb-Rosenbljum bound (see Reed and Simon [24, Thm. XIII.12] for references) due to Daubechies [2, see (2.1), (2.2) & (2.10)]. It asserts, that for a single particle Hamiltonian $T(-i\nabla) + V(x)$ (with certain conditions on T, fullfilled for the operator H_0), the absolute value of the sum $S(T+V)$ of negative eigenvalues of the operator $T+V$ is bounded as

$$S(T+V) \leq k_3 \int_{\mathbb{R}^3} d^3x\,\Big(\int_0^{W(x)} du\,[T^{-1}(u)]^3\Big)$$

with $W = \max\{0, -V\}$ and $k_3 = 1/(6\pi^2)$, whereas the number of these bound states, $N(T+V)$, is bounded as

$$N(T+V) \leq k_3 \int_{\mathbb{R}^3} d^3x\,[T^{-1}(W(x))]^3.$$

We have in our case, that

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

and so

$$F(s) = \int_0^s du\,[T^{-1}(u)]^3 = \int_0^s (t^2 + 2t)^{3/2}\,dt$$
$$= \int_0^s (2t)^{3/2}\Big(1 + \frac{t}{2}\Big)^{3/2}\,dt.$$

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

$$\Big(1 + \frac{t}{2}\Big)^{3/2} = 1 + \frac{3}{4}t + \frac{3}{32}t^2 - \frac{3t^3}{128}\int_0^1 (1-s)^2\big(1 + \frac{st}{2}\big)^{-3/2}\,ds$$
$$\le 1 + \frac{3}{4}t + \frac{3}{32}t^2$$

since the last term is negative for $t \ge 0$. That is, for $s \ge 0$:

$$F(s) \le \int_0^s (2t)^{3/2}\Big(1 + \frac{3}{4}t + \frac{3}{32}t^2\Big)\,dt$$
$$= 2\sqrt{2}\left\{\frac{2}{5}s^{5/2} + \frac{3}{14}s^{7/2} + \frac{1}{48}s^{9/2}\right\}.$$

In this way,

$$S(H_0 + V) \qquad \text{(E.14)}$$
$$\le k_3 \int_{\mathbb{R}^3} d^3x\, 2\sqrt{2}\left\{\frac{2}{5}W(x)^{5/2} + \frac{3}{14}W(x)^{7/2} + \frac{1}{48}W(x)^{9/2}\right\}$$

and

$$N(H_0 + V) \qquad \text{(E.15)}$$
$$\le k_3 \int_{\mathbb{R}^3} d^3x\, 2\sqrt{2}\left\{W(x)^{3/2} + \frac{3}{4}W(x)^{5/2} + \frac{3}{32}W(x)^{7/2}\right\}.$$

The problem is that both of the integrals in (E.14) and (E.15) are divergent for the potential

$$V_\kappa = -\frac{\delta}{|x|} + \kappa. \qquad \text{(E.16)}$$

In order to deal with this divergence, we need to 'pull the Coulomb tooth' (an expression apparently coined by Lieb and Simon in [21, sec. III.4]).

To this end, we need the following formula from Lieb and Yau [23, p. 186; here, $m = 1$]:

$$\big(f, (\sqrt{p^2+1} - 1)f\big)$$
$$= \frac{1}{4\pi^2}\iint |f(x) - f(y)|^2 |x-y|^{-2} K_2(|x-y|)\,d^3x\,d^3y.$$

Here, K_2 is a modified Bessel-function. (Note, that the formula as it stands in Lieb and Yau [23] is incomplete: one need to substract the 'rest energy' $m = 1$ from the square root to get the right formula. This is also 'morally' right, since this is the true *kinetic* energy; see Sørensen [40, App. B] for more details). We also need the following theorem from Lieb and Yau [23, Theorem 7]:

Theorem E.3 (Kinetic energy in balls). *Let B be a ball of radius D centered at $z \in \mathbb{R}^3$ and let $f \in L^2(B)$. Define*

$$(f, |p|f)_B \equiv \frac{1}{2\pi^2} \int_B \int_B |f(x) - f(y)|^2 |x - y|^{-4}\, d^3x\, d^3y \tag{E.17}$$

and assume this is finite. Then

$$(f, |p|f)_B \geq D^{-1} \int_B Q(|x - z|/D) |f(x)|^2\, d^3x, \tag{E.18}$$

where $Q(r)$ is defined for $0 < r \leq 1$ by

$$Q(r) = 2/(\pi r) - Y_1(r)$$

for some continuous function Y_1 satisfying $Y_1(r) \leq c_1 = 1.56712$ for $r \leq 1$.

The idea is to explore the fact, that $K_2(x) \sim 2/x^2$ for $x \sim 0$ (see Abramowitz and Stegun [1, 9.6.9, p. 375]) to obtain a similar result for $\sqrt{p^2+1} - 1$. More precisely, (see 9.6.11 loc. cit.)

$$\begin{aligned} K_2(x) &= \frac{1}{2}\Big(\frac{1}{2}x\Big)^{-2}\Big(1 - \frac{1}{4}x^2\Big) - \ln(\tfrac{1}{2}x) I_2(x) \\ &\quad + \frac{1}{2}\Big(\frac{1}{2}x\Big)^2 \sum_{k=0}^{\infty} \big\{\psi(k+1) + \psi(2+k+1)\big\} \frac{(\frac{1}{4}x^2)^k}{k!(2+k)!} \\ &\geq \frac{2}{x^2} - \frac{1}{2} - \frac{\gamma}{16}x^2, \end{aligned}$$

since, $\psi(n) = \Gamma'(x)/\Gamma(x)$ satisfies $\psi(n) > 0$ for $n \geq 2$ and $\psi(1) = -\gamma$ (Euler's constant — see 6.3.1, p. 258 loc. cit.) and the modified Bessel-function I_2 has the asymptotic behaviour $I_2 \sim x^2/24$, $x \sim 0$ (see 9.6.7. loc. cit.). This means, that

$$\frac{x^2 K_2(x)}{2} \geq 1 - \frac{x^2}{4} - \frac{\gamma}{32}x^4.$$

Because the postitive root of $\frac{\gamma}{32}y^2 + \frac{1}{4}y - \epsilon = 0$ is

$$y_0 = \tfrac{4}{\gamma}(\sqrt{1 + 2\epsilon\gamma} - 1) \geq \frac{4}{\gamma}(\epsilon\gamma - \epsilon^2\gamma^2) = 4\epsilon(1 - \gamma\epsilon),$$

(note, that we now need $\epsilon < 1/\gamma \approx 1.73$) we have, that

$$y \leq 4\epsilon(1 - \gamma\epsilon) \quad \Rightarrow \quad 1 - \frac{y}{4} - \frac{\gamma}{32}y^2 \geq 1 - \epsilon$$

and so

$$x \leq 2\sqrt{\epsilon}(1 - \gamma\epsilon)^{1/2} \equiv r(\epsilon) \quad \Rightarrow \quad \frac{x^2 K_2(x)}{2} \geq 1 - \epsilon. \tag{E.19}$$

Defining $B = B(r(\epsilon)/2)$, this means that

$$\begin{aligned}
&\big(f,(\sqrt{p^2+1}-1)f\big)_B \\
&\quad \equiv \frac{1}{2\pi^2}\int_B\int_B |f(x)-f(y)|^2|x-y|^{-4} \\
&\qquad\qquad\qquad \times \left(\frac{|x-y|^2K_2(|x-y|)}{2}\right) d^3x\, d^3y \\
&\quad \geq \big(1-\epsilon\big)\ \frac{1}{2\pi^2}\int_B\int_B |f(x)-f(y)|^2|x-y|^{-4}\, d^3x\, d^3y \\
&\quad = \big(1-\epsilon\big)\ \big(f,|p|f\big)_B
\end{aligned}$$

since, by (E.19),

$$\begin{aligned}
x, y\in B \quad &\Rightarrow \quad |x-y|\leq r(\epsilon) \\
&\Rightarrow \quad \frac{1}{2}|x-y|^2K_2(|x-y|)\geq 1-\epsilon.
\end{aligned}$$

This means, by Theorem E.3 (with $z=0$) that

$$\begin{aligned}
&\frac{1}{1-\epsilon}\big(f,(\sqrt{p^2+1}-1)f\big)-\big(f,\frac{2}{\pi}\frac{1}{|x|}f\big)_B \\
&\quad\geq \frac{1}{1-\epsilon}\big(f,(\sqrt{p^2+1}-1)f\big)_B-\big(f,\frac{2}{\pi}\frac{1}{|x|}f\big)_B \\
&\quad\geq \big(f,|p|f\big)_B-\big(f,\frac{2}{\pi}\frac{1}{|x|}f\big)_B\geq -\big(f,\frac{2}{r(\epsilon)}Y_1(2|x|/r(\epsilon))f\big)_B.
\end{aligned} \tag{E.20}$$

In this way, given a $\delta<2/\pi$, let ϵ be such that $\delta\leq 2(1-\epsilon)^2/\pi$ (that is, $\epsilon\leq 1-\sqrt{\delta\pi/2}$). Define the corresponding number $r(\epsilon)$ as in (E.19), and the ball $B=B(r(\epsilon)/2)$, then by the estimate in (E.20), we get (with χ_B the characteristic function of the ball B) that (see (E.16))

$$\begin{aligned}
&H_0+V_\kappa=\sqrt{p^2+1}-1-\frac{\delta}{|x|}+\kappa \\
&=(1-\epsilon)\left(\sqrt{p^2+1}-1-\frac{2(1-\epsilon)}{\pi}\frac{1}{|x|}\chi_B\right)+\kappa \\
&\qquad+\left(\frac{2(1-\epsilon)^2}{\pi}-\delta\right)\frac{1}{|x|}\chi_B+\epsilon\Big(\sqrt{p^2+1}-1-\frac{\delta/\epsilon}{|x|}\chi_{\mathbb{R}^3\setminus B}\Big) \\
&\geq \epsilon\left(\sqrt{p^2+1}-1-\frac{2(1-\epsilon)^2}{\epsilon r(\epsilon)}Y_1\Big(\frac{2|x|}{r(\epsilon)}\Big)\chi_B-\frac{\delta/\epsilon}{|x|}\chi_{\mathbb{R}^3\setminus B}+\frac{\kappa}{\epsilon}\right) \\
&\geq \epsilon\left(\sqrt{p^2+1}-1-\frac{2c_1(1-\epsilon)^2}{\epsilon r(\epsilon)}\chi_B-\frac{\delta/\epsilon}{|x|}\chi_{\mathbb{R}^3\setminus B}+\frac{\kappa}{\epsilon}\right)
\end{aligned}$$

with c_1 as in Theorem E.3. Using that the operator inequality $T_1 \geq \epsilon\, T_2$ implies that $N(T_1) \leq N(T_2)$ and $S(T_1) \leq \epsilon\, S(T_2)$, we get that

$$\begin{aligned} \sum_{e_j<-\kappa} |e_j| = \sum_{e_j+\kappa<0} |e_j| &\leq \Bigg(\sum_{e_j+\kappa<0} |e_j+\kappa| \Bigg) + \kappa \Bigg(\sum_{e_j+\kappa<0} 1 \Bigg) \\ &= S(H_0+V_\kappa) + \kappa\, N(H_0+V_\kappa) \\ &\leq \epsilon\, S(H_0+\tilde{V}_\kappa) + \kappa\, N(H_0+\tilde{V}_\kappa) \end{aligned} \tag{E.21}$$

with

$$\tilde{V}_\kappa(x) = \begin{cases} -\frac{2c_1(1-\epsilon)^2}{\epsilon r(\epsilon)} + \frac{\kappa}{\epsilon} & \text{for } |x| \leq \frac{r(\epsilon)}{2} \\ -\frac{\delta/\epsilon}{|x|} + \frac{\kappa}{\epsilon} & \text{for } |x| \geq \frac{r(\epsilon)}{2}. \end{cases}$$

In this way,

$$\begin{aligned} &\int_{\mathbb{R}^3} d^3x\, \big(\max\{-\tilde{V}_\kappa(x),0\}\big)^{n/2} \\ &= 4\pi \int_0^{\frac{r(\epsilon)}{2}} \left(\frac{2c_1(1-\epsilon)^2}{\epsilon r(\epsilon)} - \frac{\kappa}{\epsilon} \right)^{n/2} t^2\, dt + 4\pi \int_{\frac{r(\epsilon)}{2}}^{\delta/\kappa} \left(\frac{\delta/\epsilon}{t} - \frac{\kappa}{\epsilon} \right)^{n/2} t^2\, dt. \end{aligned}$$

Now,

$$4\pi \int_{\frac{r(\epsilon)}{2}}^{\delta/\kappa} \left(\frac{\delta/\epsilon}{t} - \frac{\kappa}{\epsilon} \right)^{n/2} t^2\, dt \leq \begin{cases} \frac{\delta^3}{\epsilon^{n/2}(3-n/2)} \kappa^{n/2-3}, & n<6 \\ (\delta/\epsilon)^{n/2} \left(\frac{2}{r(\epsilon)}\right)^{n/2-3}, & n>6 \end{cases}$$

by the change of variables $y = \kappa|x|/\delta$, whereas

$$\begin{aligned} &4\pi \int_0^{\frac{r(\epsilon)}{2}} \left(\frac{2c_1(1-\epsilon)^2}{\epsilon r(\epsilon)} - \frac{\kappa}{\epsilon} \right)^{n/2} t^2\, dt \\ &\qquad\qquad \leq \frac{4\pi}{3} \left(\frac{r(\epsilon)}{2} \right)^3 \left(\frac{2c_1(1-\epsilon)^2}{\epsilon r(\epsilon)} \right)^{n/2}, \end{aligned}$$

and so, since $\kappa \in]0,1]$, we have that (for some C; here we lost track of constants...)

$$\int_{\mathbb{R}^3} d^3x\, \big(\max\{-\tilde{V}_\kappa,0\}\big)^{n/2} \leq C\, \kappa^{-1/2} \quad \text{for all } n \in \{5,7,9\}$$

whereas (for some C')

$$\int_{\mathbb{R}^3} d^3x\, \big(\max\{-\tilde{V}_\kappa,0\}\big)^{n/2} \leq C'\, \kappa^{-3/2} \quad \text{for all } n \in \{3,5,7\}.$$

By (E.14) and (E.15) this means, that

$$\sum_{e_j<-\kappa} |e_j| \leq \epsilon\, S(H_0+\tilde{V}_\kappa) + \kappa\, N(H_0+\tilde{V}_\kappa) \leq C_5 \frac{1}{\sqrt{\kappa}}$$

and

$$\sum_{e_j<-\kappa} 1 = \sum_{e_j+\kappa<0} 1 \leq N(H_0 + \tilde{V}_\kappa) \leq C_6 \frac{1}{\kappa\sqrt{\kappa}}$$

for some constants C_5 and C_6, that only depend on δ (and the choice of ϵ). This proves Lemma E.2. □

Appendix F. An integral representation of $g(B)$

In this appendix we will make the necessary calculations to prove the formula (B.71) on the level of functions. The result for self-adjoint operators follows by the spectral theorem.

Lemma F.1. *For $g \in C_0^\infty(\mathbb{R})$, all $n \geq 2$ and all $\xi \in \mathbb{R}$ we have*

$$\begin{aligned} g(\xi) = &\sum_{j=0}^{n-1} \frac{1}{\pi j!} \int_{\mathbb{R}} \partial^j g(\lambda) \operatorname{Im}[i^j(\xi - \lambda - i)]\, d\lambda \\ &+ \frac{1}{\pi(n-1)!} \int_0^1 \tau^{n-1}\, d\tau \int_{\mathbb{R}} \partial^n g(\lambda) \operatorname{Im}[i^j(\xi - \lambda - i\tau)]\, d\lambda. \end{aligned}$$

Proof. To prove this, we need two things. First of all, we need to extend g into the complex plane: Let for λ and τ in $\mathbb{R}$:

$$\tilde{g}(\lambda + i\tau) = \sum_{j=0}^{n-1} \frac{\partial^j g(\lambda)(i\tau)^j}{j!}. \tag{F.1}$$

Think of this as a formal Taylor-expansion. We also need the fundamental solution for the Laplacian in $\mathbb{R}^2$: Let $E(x) = (2\pi)^{-1}\log|x|$, then $\Delta E = \delta_0$, in distribution sense (see Hörmander [15, Thm. 3.3.2]). Now we are ready, the rest is pure calculus: Note, that with

$$\partial_{\bar{z}} = \frac{1}{2}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right) \text{ and } \partial_z = \frac{1}{2}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right) \tag{F.2}$$

we have $4\Delta = \partial_{\bar{z}}\partial_z$. By the above, for ξ real and $K \subset \mathbb{C}$ a 'nice' compact set (since $\tilde{g} \in C_0^\infty(\mathbb{R}^2)$)

$$\begin{aligned} g(\xi) = \tilde{g}(\xi) &= \langle \delta_\xi, \tilde{g}\rangle = \langle (2\pi)^{-1}\Delta \log|\cdot - \xi|, \tilde{g}\rangle \\ &= \frac{1}{8\pi}\int_K \tilde{g}(z)\partial_{\bar{z}}\partial_z \log|z-\xi|\, dz\, d\bar{z}. \end{aligned}$$

Now,

$$\begin{aligned} 2\,\partial_{\bar{z}}\partial_z \log|z-\xi| &= \partial_{\bar{z}}\partial_z \log|z-\xi|^2 \\ &= \partial_{\bar{z}}\partial_z \log\big\{(z-\xi)(\bar{z}-\xi)\big\} = \partial_{\bar{z}}\left(\frac{1}{z-\xi}\right) \end{aligned}$$

and so, by Stoke's theorem, we have

$$g(\xi) = \frac{1}{4\pi}\int_{\partial K} \frac{\tilde{g}(z)\, dz}{z-\xi} - \frac{1}{4\pi}\int_K \frac{\partial_{\bar{z}}\tilde{g}(z)}{z-\xi}\, d\bar{z}\, dz.$$

A straightforward calculation, using (F.1) and (F.2) with $z = \lambda + i\tau$ shows, that

$$\partial_{\bar{z}} \tilde{g}(z) = \frac{1}{2} \frac{\partial^n g(\lambda)(i\tau)^{n-1}}{(n-1)!}.$$

Choose now $K \subset \mathbb{C}$ to be a rectangle, $K = [-C, C] \times i[-1, 1]$, C large, such that supp $g \subset [-C, C]$. Then, noticing that $\tilde{g}$ is zero on the vertical sides of K, we get (since $d\bar{z}\, dz = 2\, d\tau\, d\lambda$)

$$\begin{aligned}
g(\xi) = & \frac{1}{2\pi} \int_{-C}^{C} \sum_{j=0}^{n-1} \frac{\partial^j g(\lambda)(i(-1))^j}{j!} \frac{1}{\lambda - i - \xi}\, d\lambda \\
& - \frac{1}{2\pi} \int_{-C}^{C} \sum_{j=0}^{n-1} \frac{\partial^j g(\lambda)(i)^j}{j!} \frac{1}{\lambda + i - \xi}\, d\lambda \\
& - \frac{1}{4\pi} \int_{-1}^{1} d\tau \int_{-C}^{C} dt \left(\frac{\partial^n g(\lambda)(i\tau)^{n-1}}{(n-1)!} \frac{1}{\lambda + i\tau - \xi} \right) \\
= & \sum_{j=0}^{n-1} \frac{1}{\pi j!} \int_{\mathbb{R}} \partial^j g(\lambda)\, \mathrm{Im}[i^j(\xi - \lambda - i)]\, d\lambda \\
& + \frac{1}{\pi(n-1)!} \int_0^1 \tau^{n-1}\, d\tau \int_{\mathbb{R}} \partial^n g(\lambda)\, \mathrm{Im}[i^j(\xi - \lambda - i\tau)]\, d\lambda.
\end{aligned}$$

The last equality follows from splitting the last integral in integrations over positive, resp. negative τ, making a change of variables and collecting the terms. □

Appendix G. A Numerical Computation

The following is the Maple©-code that generated the plot in the introduction.

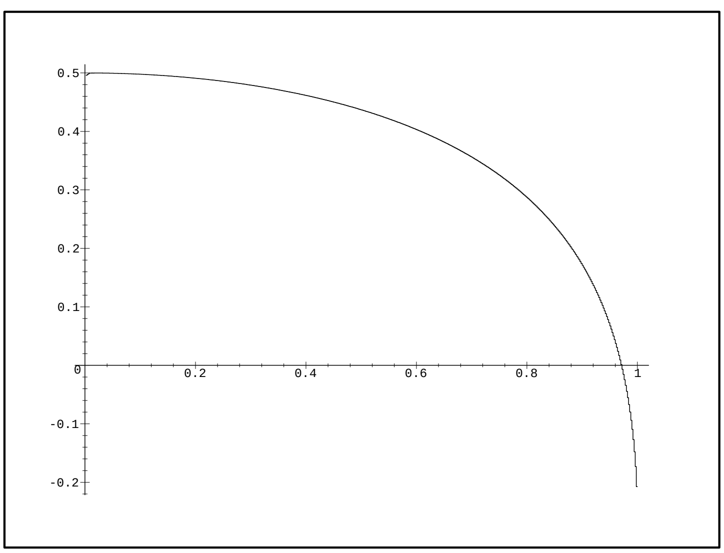
$EnergyDirac := \mathbf{proc}(d,\ n,\ k)$
  $\mathrm{evalf}((1/(1 + d^2/(n + \mathrm{sqrt}(k^2 - d^2))^2)^{(1/2)} - 1)/d^2)$
end

$EnergySchr := \mathbf{proc}(d,\ n,\ k)\ \mathrm{evalf}(-1/2 \times 1/(n+k)^2)$ **end**

```
EnergyDiff := proc(d, N)
    local n, k;
    global dE;
        dE := 0 ;
        for k while k < N do
            dE := dE + EnergyDirac(d, 0, k) − EnergySchr(d, 0, k) ;
            for n while n + k < N do
                dE := dE + EnergyDirac(d, n, k) − EnergySchr(d, n, k)
            od
        od;
        dE := dE + 1/2 ;
        dE
    end
```

```
PlotEnergyDiff := proc(n, N)
    local i, points;
        points := [
            seq([[i/n, EnergyDiff(i/n, N)], [(i + 1)/n, EnergyDiff(i/n, N)]], i = 1..n − 1)]
            ;
        points := map(op, points) ;
        PLOT(CURVES(points))
    end
```

```
> PlotEnergyDiff(700,40);
```



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THE LARGE - Z BEHAVIOUR OF PSEUDO-RELATIVISTIC ATOMS

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ABSTRACT. This paper is my progress-report for the qualifying exam after the 'del A' of the PhD-program. It treats the large Z-behaviour of the ground state energy of atoms with electrons having relativistic kinetic energy $\sqrt{p^2c^2 + m^2c^4} - mc^2$.

CONTENTS

1. INTRODUCTION

As a model for a relativistic atomic with atom number Z and N electrons, we wish to consider the operator

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

This dimensionless expression for the Hamiltonian of a relativistic atom is developed in appendix C.

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This model has been much studied over the past twenty years. Stability in the case $N = 1$ was proved independently by Herbst [7] and Weder [19]. The 'Stability of Matter' for the model was first proved by Conlon [1], later by Fefferman and de la Llave [5], and also by Lieb and Yau [15]; see the latter for an overview. This paper relies to a great extent on the work by Lieb and Yau.

It is well-known that the operator H_{rel} is bounded from below on $C_0^\infty(\mathbb{R}^{3N})$ if, and only if, $Z\alpha \leq \frac{2}{\pi}$. 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. Due to the upper bound on Z however, this is not possible here. To overcome this problem, we consider

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

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

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

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. 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

$$\inf\ \mathrm{Spec}_{\mathcal{H}_F} H_{rel} = \inf_{\{\psi\in\mathcal{C}\,|\,\|\psi\|=1\}}\langle\psi, H_{rel}\psi\rangle$$

Our main result will be the following:

Theorem 1.1. *Let δ be fixed, $0 \leq \delta \leq 2/\pi$, and let H_{rel} and $E_{N=Z}(Z,\delta)$ be as above. Then one has:*

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

where $C_{TF}Z^{7/3}$ is the Thomas-Fermi energy of the atom.

This shows that, to leading order, the ground-state energy of a relativistic atom is given by the semi-classical Thomas-Fermi energy approximation, as it is for the non-relativistic atom (Note that the case $\delta = \frac{2}{\pi}$ is included). This was first proved by Lieb and Simon [12]; see also Lieb [9]. This expresses the fact that for large atoms the majority of the electrons are non-relativistic.

The aim of the sequence of my work is to try to understand the relativistic corrections to the energy of the atom. These are expected to appear in the lower order terms in the asymptotic expansion (in Z) of $E_{N=Z}(Z,\delta)$. More precisely, we expect:

Conjecture 1.2. For all δ, $0 \leq \delta < \frac{2}{\pi}$, there is a constant $s(\delta)$ such that

$$E_{N=Z}(Z,\delta) = C_{\mathrm{TF}} Z^{7/3} + s(\delta) Z^2 + o(Z^2) \quad , \quad Z \to \infty \tag{1.2}$$

where $s(\delta)$ satisfies

$$\lim_{\delta \to 0} s(\delta) = 1/2. \tag{1.3}$$

For non-relativistic atoms, this asymptotic limit is well-known; the second term in (1.2) is known as the 'Scott-correction' and is equal to $Z^2/2$. This was conjectured by Scott [16] and proved by Hughes [8] and Siedentop and Weikard [17, 18]. The non-relativistic case is what makes us expect (1.3), since, in some sense, the limit as $\delta \to 0$ is the non-relativistic limit. The proof of the theorem will be by semi-classical eigenvalue estimates, while the proof of the conjecture is expected to involve Fourier Integral methods. It would also, if the conjecture holds, be interesting to study the function $s(\delta)$ and compare this both with numerical (Dirac-Hartree-Fock) calculations of the energy of relativistic atoms, and with experimental results. Mass-spectroscopic measurements of the energy exists for $Z < 25$.

The proof of the theorem will be by finding upper and lower bounds on $E_{N=Z}(Z,\delta)$. As noted in appendix C, the relativistic kinetic energy is always lower than the non-relativistic one:

$$\sqrt{p^2\alpha^{-2} + \alpha^{-4}} - \alpha^{-2} = \alpha^{-2}\left(\sqrt{1+(\alpha p)^2} - 1\right) \leq \frac{p^2}{2}. \tag{1.4}$$

(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 $p^2/2$). This means, that all upper bounds derived earlier for the non-relativistic operator

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

will still be valid; 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 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 an analogue of the IMS Localisation Formula for the Schrödinger operator, see [2, p.27]. This formula has already been developed by Lieb and Yau in [15] for both the operator $\sqrt{-\Delta+\alpha^{-2}}$ and the hyper relativistic kinetic energy $|p|$. This is essentially done by finding the integral kernels of these operators. For $\sqrt{-\Delta+\alpha^{-2}}$, 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 the appendix A. The localisation error, given by a bounded operator $L^{(\alpha)}$ expressed as an integral operator involving K_2 is then estimated. 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.

Coming to the localised energy, we have to estimate the kinetic energy close to the nucleus. This is the region, where the electrons are relativistic, since this is the high-energy region, 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. The problem is solved by a clever choice of parameters in an estimate by Lieb and Yau in [15] 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 essentially the same idea as Lieb did in the classical case, see [10], 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 [14], but the error obtained there is too rough for our purposes. We therfore develop 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 by an additional cut-off. The energy in this core is estimated by a generalised version of the Lieb-Thirring inequality, proved by Daubechies in [3]. Also the other part of the previously mentioned two terms of the localised operator $L^{(\alpha)}$ is estimated in this way.

Finally we relate 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 $\sqrt{-\Delta+\alpha^{-2}}$ to the classical one, $p^2/2$, getting errors of the desired order.

3. Reduction to a one-particle problem

We will use the notation

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

With this, since we wish to consider α as the free parameter, the relevant order of all error terms will be $o(\alpha^{-4/3})$, since $\delta = Z\alpha$ is fixed and since the ground state energy of H_{rel} is to be proved to be of leading order $Z^{7/3}$. We apologise to the reader for the inconvenience of this unfamiliar choice, but since we started out by using this approach, we will stick to this notation in this paper. 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 now 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:

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

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 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:

$$\begin{aligned}H &= \sum_{i=1}^N\Big\{\sqrt{p_i^2+\alpha^{-2}}-\alpha^{-1}-\frac{\delta}{|x_i|}\Big\}+\sum_{1\le i<j\le N}\frac{\alpha}{|x_i-x_j|}\\ &\ge\sum_{i=1}^N\Big\{\sqrt{p_i^2+\alpha^{-2}}-\alpha^{-1}-\frac{\delta}{|x_i|}+\alpha\,\rho*\phi_a*|x_i|^{-1}\Big\} \qquad (3.1)\\ &\qquad -\frac{\alpha}{2}\iint\frac{\rho(x)\rho(y)}{|x-y|}\,d^3x\,d^3y-\alpha\,c(\phi)Na^{-1}.\end{aligned}$$

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

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

where $m_i\in L^2(\mathbb{R}^3), i=1,\ldots,N$ are orthonormal. Note also that since $C_0^\infty(\mathbb{R}^3)$ is a core for the operator $\sqrt{p^2+\alpha^{-2}}-\alpha^{-1}-\delta/|x|$ (see Herbst [7]), 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 find 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 (3.1) 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 [15], a partition of unity (see also Cycon, Froese, Kirsch and Simon [2, definition 3.1]). For $\beta \in (0, \frac{1}{2})$, let θ_1 and θ_2 be positive smooth functions on $\mathbb{R}_+$, $0 \le \theta_i \le 1$, such that

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

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

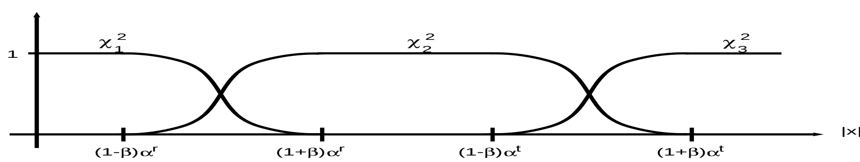
and such that $\theta_1(\xi)^2 + \theta_2(\xi)^2 = 1$ for all $\xi \in \mathbb{R}_+$. Now define, with $8/9 < r < 1$ and $1/3 < t < 2/3$ (these choices of parameters are governed by the later analysis), the following partition of unity in $\mathbb{R}^3$:

$$\chi_1(x) = \theta_1\Big(\frac{|x|}{\alpha^r}\Big)$$

$$\chi_2(x) = \theta_1\Big(\frac{|x|}{\alpha^t}\Big)\, \theta_2\Big(\frac{|x|}{\alpha^r}\Big)$$

$$\chi_3(x) = \theta_2\Big(\frac{|x|}{\alpha^t}\Big)$$

Then we have the following picture, at least for α sufficiently small:



.

Figure 1. *The partition of unity.*

According to Lieb and Yau [15, Theorem 9; α^{-1} corresponds to m] we have for $f \in C_0^\infty(\mathbb{R}^3)$, that

$$(f, \sqrt{p^2+\alpha^{-2}}f) = \sum_{j=1}^{3}(f, \chi_j\sqrt{p^2+\alpha^{-2}}\chi_j f) - (f, L^{(\alpha)}f) \qquad (4.1)$$

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 the derivation of this, see 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

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

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

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 $L^{(\alpha)}$, whose kernel is calculated in appendix A:

$$
L^{(\alpha)}(x,y) = \sum_{j=1}^{3} L_j^{(\alpha)}(x,y)
$$

where

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

We shall start by localising this operator, thereby splitting it it into twelve terms (!) which we will then treat individually. The 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:

$$
\begin{aligned}
L_j^{(\alpha)}(x,y) \;\; = \;\; & \chi_+(x) L_j^{(\alpha)}(x,y) \chi_+(y) + \chi_+(x) L_j^{(\alpha)}(x,y) \chi_-(y) \\
& + \chi_-(x) L_j^{(\alpha)}(x,y) \chi_+(y) + \chi_-(x) L_j^{(\alpha)}(x,y) \chi_-(y).
\end{aligned}
$$

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 on*

$$\text{supp } \chi_+(x) L_j^{(\alpha)}(x,y)\chi_-(y)$$

one has:

$$|x| > al \quad , \quad |y| < bl \quad , \quad \gamma \equiv 1 - \frac{b}{a} > 0\,.$$

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

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

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 is symmetric in x and y.

Proof. By the assumption, we have that

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

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 $(\chi_j(x) - \chi_j(y))^2 \leq 1$, we get, pointwise:

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

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

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

Both of these terms can be estimated using the Cauchy-Schwartz inequality. For the first, we get

$$\int |f(y)|\, \chi_-(y)\, d^3y \leq \|f\|_2 \, \|\chi_-\|_2 = \sqrt{\frac{32\pi}{3}} l^{3/2} \|f\|_2$$

and for the second

$$\begin{aligned}
&\int |f(x)|\, \chi_+(x) \frac{K_2(\alpha^{-1}\gamma|x|)}{|x|^2}\, d^3x \\
&\qquad\qquad \leq \|f\|_2 \left(\int \left(\chi_+(x) \frac{K_2(\alpha^{-1}\gamma|x|)}{|x|^2} \right)^2 d^3x \right)^{1/2}.
\end{aligned}$$

Using the estimate (B.7) in appendix A on K_2, we now get the estimate

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

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 the following (remember, that $l=\alpha^r$):

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

where $C=(8\sqrt{2})\Big/(\pi\gamma\sqrt{3\gamma})$ and

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

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

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

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:

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

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 the lemma and therefore are $o(e^{-\epsilon\alpha^{r-1}})$ for some $\epsilon>0$:

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

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 need the Mean Value Theorem in $\mathbb{R}^3$:

Theorem 5.3. *Let $\phi : \mathbb{R}^3 \to \mathbb{R}$ be C^1, and let x and y be in $\mathbb{R}^3$. Then there exists $\xi \in Lin]x, y[$ (the line from x to y) such that*

$$\nabla\phi(\xi) \cdot (x - y) = \phi(x) - \phi(y).$$

Proof. This is seen by parametrising $\mathrm{Lin}[x, y]$ by $\gamma(t) = tx + (1-t)y$, $t \in [0, 1]$ and then using the normal Mean Value Theorem on the function $\phi \circ \gamma : [0, 1] \to \mathbb{R}$. $\square$

In this way, $(\chi_j(x) - \chi_j(y))^2 \leq \|\nabla\chi_j\|_\infty^2 |x - y|^2$. Note that for the four remaining terms,

$$\begin{array}{ll} \chi_+ L_2^{(\alpha)} \chi_+ & \qquad \chi_- L_1^{(\alpha)} \chi_- \\ \chi_+ L_3^{(\alpha)} \chi_+ & \qquad \chi_- L_2^{(\alpha)} \chi_- \end{array}$$

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

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

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

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

For two of these terms, $\chi_+ L_2^{(\alpha)} \chi_+$ and $\chi_+ L_3^{(\alpha)} \chi_+$, this is sufficient, since

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

and since $t < 2/3$, one gets

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

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, 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 supp χ_-. Using this, we obtain (since $\chi_-\chi_1 = \chi_1$):

$$\begin{aligned}&\sum_{i=1}^{N}(m_i, \chi_-(L_1^{(\alpha)} + L_2^{(\alpha)})\chi_- m_i)\\ &\qquad \leq C\,\alpha^{1-2r}\Big(\sum_{i=1}^{N}(\chi_1 m_i, \chi_1 m_i) + \sum_{i=1}^{N}(\chi_2 m_i, \chi_-\chi_2 m_i)\Big) \qquad (5.1)\end{aligned}$$

where

$$\begin{aligned}C &= \frac{3}{2}(c_1 + c_2)\\ c_1\alpha^{-2r} &= \sup_{|x|<2l} |\nabla\chi_1(x)|^2 = \|\nabla\chi_1\|_\infty^2\\ c_2\alpha^{-2r} &= \sup_{|x|<2l} |\nabla\chi_2(x)|^2.\end{aligned}$$

The two terms in (5.1) 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 will estimate the energy at the nucleus, that is, the term

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

Also, half of the remaining term (5.1) 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 of (6.1) by dropping this term. The remaining expression will be treated by using the following result on the hyper relativistic operator $|p|$ by Lieb and Yau [15, Theorem 11]:

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

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

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 $B_R = \{x \mid |x| \leq R\}$. Then

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

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 [11]. In our situation, $q = 2$. For our purpose, let Π be the projection on $\mathrm{span}\{m_i \mid i = 1, \ldots N\}$, then Π is a density matrix as above, and

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

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

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

since $\sqrt{p^2 + \alpha^{-2}} - \alpha^{-1} \geq |p| - \alpha^{-1}$ and $\delta \leq 2/\pi$. Including the first term in (5.1) we now have

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

where $c = 44\int_0^\infty |\theta_1(t)|^2 t^2\, dt$. The second inequality is valid for α small enough, since $r < 1$, so that $\alpha^{2(1-r)} \to 0$ for $\alpha \to 0$. Now $3r - 4 > -4/3$, so that the last term 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

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

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 [13]), proved by Daubechies in [3, 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*

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

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,

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

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 (5.1). 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

$$\begin{aligned}\left(1+\frac{\alpha t}{2}\right)^{3/2} &= 1+\frac{3\alpha}{4}t+\frac{3\alpha^2}{32}t^2-\frac{3\alpha^3t^3}{128}\int_0^1(1-s)^2\big(1+\frac{s\alpha t}{2}\big)^{-3/2}\,ds\\ &\le 1+\frac{3\alpha}{4}t+\frac{3\alpha^2}{32}t^2 \qquad (7.3)\end{aligned}$$

since the last term is negative for $t \ge 0$. That is, for $s \ge 0$:

$$\begin{aligned}F(s) &\le \int_0^s \big(\frac{2t}{\alpha}\big)^{3/2}\big(1+\frac{3\alpha}{4}t+\frac{3\alpha^2}{32}t^2\big)\,dt\\ &= \big(\frac{2}{\alpha}\big)^{3/2}\Big\{\frac{2}{5}s^{5/2}+\frac{3\alpha}{14}s^{7/2}+\frac{\alpha^2}{48}s^{9/2}\Big\}.\end{aligned}$$

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

$$\sum_{i=1}^N (m_i,\chi_2\{T(p)-V(x)\}\chi_2 m_i)$$

and

$$C\,\alpha^{1-2r}\sum_{i=1}^N(\chi_2 m_i,\chi_-\chi_2 m_i).$$

In order to do so, note that on supp $\chi_-\chi_2$ we have

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

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

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

with $\tilde V(x)=\chi_2(x)V(x)$. Letting (e_j,g_j) be the negative eigenvalues and corresponding orthonormal eigenvectors for the operator $T(p)-$

$2\tilde{V}(x)$ as before, we then have

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

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 $T(p)-2\tilde{V}(x)$, in the limit $N\to\infty$, we now reach

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

where $\bar{C}=64\pi\tilde{C}\delta^{5/2}$. 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

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

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 [14, 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 $N = \lambda Z = \lambda\delta\alpha^{-1}$:

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

which is also $o(\alpha^{-4/3})$. 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 $\sqrt{p^2 + \alpha^{-2}} - \alpha^{-1}$, one then has the formulae

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

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 $\phi_{\alpha^s} = g_\alpha^2$):

$$\begin{aligned}
&\sum_{i=1}^{N}(m_i, \chi_3\{T(p) - V(x) + \alpha\,\rho * \phi_a * |x|^{-1}\}\chi_3 m_i)\\
&\quad= \sum_{i=1}^{N}(m_i, \chi_3\{T(p) - \tilde{V}(x) * \phi_{\alpha^s} + \frac{\delta}{|x|} * \phi_{\alpha^s} - \frac{\delta}{|x|}\}\chi_3 m_i)\\
&\quad= \sum_{i=1}^{N}(m_i, \chi_3\{T(p) - \tilde{V}(x) * \phi_{\alpha^s}\}\chi_3 m_i)\\
&\quad= \frac{1}{(2\pi)^3}\iint d^3p\, d^3q\, (\tilde{T}(p) - \tilde{V}(q))\Big(\sum_{i=1}^{N}|(m_i\chi_3, g_\alpha^{p,q})|^2\Big)\\
&\qquad - No(\alpha^{-1/3}).
\end{aligned}$$

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 $s > t$),

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

This is one of the reasons for introducing the intermediary zone by the function χ_2. Note also that $No(\alpha^{-1/3}) = o(\alpha^{-4/3})$. 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 supp $g_\alpha \subset B(0, \alpha^s)$ and 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 $\big[f\big]_\pm = \max\{\pm f, 0\}$:

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

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 $\psi \in \mathcal{H}_F = \bigwedge^N L^2(\mathbb{R}^3, \mathbb{C}^2)$:

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

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

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

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 [12] and Lieb [9]). 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, for $N \leq Z$,

$$\int \rho_{TF}^{N,Z}(x)\,d^3x = N \quad \text{and} \quad \mu(N) > 0$$

and for $N > Z$

$$\int \rho_{TF}^{N,Z}(x)\,d^3x = Z \quad \text{and} \quad \mu(N) = 0$$

(see Lieb and Simon [12, 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 scaling ([12, (2.24) p.608]) (remember, that $\lambda = N/Z$ is fixed):

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

$$V_{TF}^{N,Z}(x) = Z^{4/3} V_{TF}^{\lambda,1}(Z^{1/3}x) \equiv Z^{4/3} V_{TF}(Z^{1/3}x). \tag{8.7}$$

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

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

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,

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

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

$$
\begin{aligned}
&\iint_{|q|>\frac14\alpha^t;\ \tilde T(p)<\alpha V_{TF}^{N,Z}(q)<\alpha\frac{p^2}{2}} d^3p\, d^3q\,\big(\alpha V_{TF}^{N,Z}(q)-\tilde T(p)\big) \\
&\qquad\qquad \leq \alpha \iint_{|q|>\frac14\alpha^t;\ \tilde T(p)<\alpha V_{TF}^{N,Z}(q)<\alpha\frac{p^2}{2}} d^3p\, d^3q\, V_{TF}^{N,Z}(q)
\end{aligned}
$$

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

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

The limits in the integral means, that

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

so that with

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

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

$$(1+Y)^{3/2} \le 1+\frac{3}{2}Y+\frac{3}{8}Y^2$$

and so

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

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

$$\begin{aligned}(8.8) &\le 8\sqrt{2}\pi^2\delta^{11/3}\alpha^{-2/3}\int_W^\infty d|\omega|\,|\omega|^{-3/2}+\sqrt{2}\pi^2\delta^5\int_W^\infty d|\omega|\,|\omega|^{-5/2}\\ &\sim \alpha^{-2/3}W^{-1/2}+W^{-3/2}\sim\alpha^{-2/3}\alpha^{1/6-t/2}+\alpha^{(1-3t)/2}\\ &= o(\alpha^{-5/6})+o(\alpha^{-1/2})\end{aligned}$$

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

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

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

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

In this way, we get

$$
\begin{aligned}
&\frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac14\alpha^t;\ \alpha\frac{p^2}{2}<\alpha V_{TF}^{N,Z}(q)} d^3p\, d^3q\, \big(\tilde T(p) - \alpha V_{TF}^{N,Z}(q)\big) \\
&\geq \frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac14\alpha^t;\ \alpha\frac{p^2}{2}<\alpha V_{TF}^{N,Z}(q)} d^3p\, d^3q\, \big(\alpha\frac{p^2}{2} - \alpha^3\frac{p^4}{8} - \alpha V_{TF}^{N,Z}(q)\big) \\
&= \frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac14\alpha^t;\ \alpha\frac{p^2}{2}<\alpha V_{TF}^{N,Z}(q)} d^3p\, d^3q\, \big(\alpha\frac{p^2}{2} - \alpha V_{TF}^{N,Z}(q)\big) \\
&\qquad\qquad - \alpha^3\frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac14\alpha^t;\ \alpha\frac{p^2}{2}<\alpha V_{TF}^{N,Z}(q)} \frac{p^4}{8}\, d^3p\, d^3q.
\end{aligned}
\tag{8.9}
$$

Note, that

$$
\begin{aligned}
&\frac{1}{(2\pi)^3}\iint\limits_{|q|>\frac14\alpha^t;\ \alpha\frac{p^2}{2}<\alpha V_{TF}^{N,Z}(q)} d^3p\, d^3q\, \big(\alpha\frac{p^2}{2} - \alpha V_{TF}^{N,Z}(q)\big) \\
&= -\frac{\alpha}{(2\pi)^3}\iint\limits_{|q|>\frac14\alpha^t} d^3p\, d^3q\, \Big[\frac{p^2}{2} - \big(\frac{Z}{|q|} - \rho_{TF}^{N,Z} * |q|^{-1} - \mu(N)\big)\Big]_- \\
&\geq -\frac{\alpha}{(2\pi)^3}\iint d^3p\, d^3q\, \Big[\frac{p^2}{2} - \big(\frac{Z}{|q|} - \rho_{TF}^{N,Z} * |q|^{-1} - \mu(N)\big)\Big]_-
\end{aligned}
$$

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

$$
\begin{aligned}
\iint\limits_{|q|>\frac14\alpha^t;\ \alpha\frac{p^2}{2}<\alpha V_{TF}^{N,Z}(q)} \frac{p^4}{8}\, d^3p\, d^3q \;\leq\; &\iint\limits_{|q|>\frac14\alpha^t;\ \alpha\frac{p^2}{2}<\delta/|q|} \frac{p^4}{8}\, d^3p\, d^3q \\
&= (4\pi)^2\int_{\frac14\alpha^t}^{\infty} d|q|\, \left(|q|^2\int_0^{\sqrt{2Z/|q|}} \frac{|p|^4}{8}|p|^2\, d|p|\right) \\
&= 2\pi^2\int_{\frac14\alpha^t}^{\infty} d|q|\, \left(|q|^2\Big[t^7/7\Big]_0^{\sqrt{2Z/|q|}}\right) \\
&= \frac{2\pi^2(2Z)^{7/2}}{7}\int_{\frac14\alpha^t}^{\infty} |q|^{-3/2}\, d|q| = \frac{8\pi^2(2Z)^{7/2}}{7}\alpha^{-t/2}.
\end{aligned}
$$

Using this, we then get the following

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

Hence, since $\delta = Z\alpha$ is fixed, we have

$$
\alpha^{(6-t)/2}\ \frac{(2Z)^{7/2}}{7\pi} = \frac{8\sqrt{2}}{7\pi}\alpha^{-(1+t)/2}\delta^{7/2}
$$

which is $o(\alpha^{-4/3})$, since $t < 2/3$.

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

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

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

$$
\begin{aligned}
&\int d^3p \left[\frac{p^2}{2} - (\frac{Z}{|q|} - \rho_{TF}^{N,Z} * |q|^{-1} - \mu(N))\right]_- \qquad (8.11) \\
&= \int_{\frac{p^2}{2}<V_{TF}^{N,Z}} \left(\frac{p^2}{2} - (\frac{Z}{|q|} - \rho_{TF}^{N,Z} * |q|^{-1} - \mu(N))\right) d^3p \\
&= 2\pi \Big[t/5\Big]_0^{\sqrt{2}\left[V_{TF}^{N,Z}\right]_+^{1/2}} \\
&\quad - \frac{4\pi}{3} 2^{3/2} \left[V_{TF}^{N,Z}(q)\right]_+^{5/2} \\
&= -\frac{16\sqrt{2}\pi}{15} \left[V_{TF}^{N,Z}(q)\right]_+^{5/2}
\end{aligned}
$$

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):

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

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

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

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

Appendix A. The dimensionless operator

In this appendix we derive a dimension-less expression for relativistic atomic Schrödinger operators. Instead of setting $h = m = c = 1$ as done most-where in the literature, we keep all relevant physical constants, to reach an expression for the relativistic quantum mechanical energy. This will be given by a dimension-less operator times the relevant fundamental energy R_∞, Rydberg's constant for infinite nuclear mass, related to the Born-Oppenheimer approximation.

In relativistic mechanics, the kinetic energy of an electron with mass m and momentum p is given by

$$E_{kin} = \sqrt{p^2c^2 + m^2c^4} - mc^2.$$

In this expression, $[p] = MLT^{-1}$. Since we wish to consider the momentum p as $p = \frac{1}{i}\nabla$, where $[p] = L^{-1}$, we re-scale p with the relevant physical constants: since $[\hbar c] = ETLT^{-1} = EL$, the appropriate expression is:

$$E_{kin} = \sqrt{\hbar^2c^2p^2 + m^2c^4} - mc^2.$$

Choosing Gaußian units, in which $\varepsilon_0 = (4\pi)^{-1}$, the Coulomb energy of two charges, Z_1e and Z_2e at x_1 resp. x_2 becomes

$$E_{Coul} = \frac{Z_1Z_2e^2}{|x_1 - x_2|}.$$

Looking then at the relativistic Schrödinger operator H_{rel} of N electrons around a nucleus of charge Ze, assumed to be at rest at the origin—the so-called Born-Oppenheimer approximation—one has

$$H_{rel} = \sum_{j=1}^{N}\left\{\sqrt{\hbar^2c^2p_j^2 + m^2c^4} - mc^2 - \frac{Ze^2}{|x_j|}\right\} + \sum_{1\le i<j\le N}\frac{e^2}{|x_i - x_j|}.$$

Now look at all the relevant physical constant. Apart from h, m, c and e, there are several combinations of these that will be of our interest:

$$\alpha = \frac{e^2}{\hbar c}: \quad \text{the fine structure constant.}$$

$$a = \frac{\hbar^2}{me^2} = \frac{\hbar}{m\alpha c}: \quad \text{the Bohr radius for atomic hydrogen.}$$

$$R_\infty = \frac{1}{2}\alpha^2mc^2 = \frac{me^4}{h^2}: \quad \text{Rydberg's constant for infinite nuclear mass.}$$

We now use these relations to derive the wanted expression for H_{rel}:

$$\begin{aligned} &H_{rel} \\ &= \sum_{j=1}^{N}\left\{\sqrt{\hbar^2c^2p_j^2 + m^2c^4} - mc^2 - \frac{Ze^2}{|x_j|}\right\} + \sum_{1\le i<j\le N}\frac{e^2}{|x_i - x_j|} \\ &= R_\infty\left(\sum_{j=1}^{N}\left\{\sqrt{\alpha^{-2}a^2p_j^2 + \alpha^{-4}} - \alpha^{-2} - \frac{a^2Z}{|x_j|}\right\} + \sum_{1\le i<j\le N}\frac{a^2}{|x_i - x_j|}\right). \end{aligned}$$

Now, to get a dimension-less expression, make the change of variables

$$y_j = \frac{x_j}{a}, \quad a = \frac{\hbar^2}{me^2}.$$

This amounts to measure lengths in units of the Bohr radius. Since $p_j = \frac{1}{i}\frac{\partial}{\partial x_j}$, one gets $q_j = ap_j$, with $q_j = \frac{1}{i}\frac{\partial}{\partial y_j}$. Note, that both y_j and q_j now are dimension-less. Inserting above yields

$$H_{rel} = R_\infty \left\{ \sum_{j=1}^{N} \left\{ \sqrt{\alpha^{-2}q_j^2 + \alpha^{-4}} - \alpha^{-2} - \frac{Z}{|y_j|} \right\} + \sum_{1\le i<j\le N} \frac{1}{|y_i - y_j|} \right\}.$$

This is the desired expression for the Hamiltonian H_{rel} with relativistic kinetic energy. To get the 'classical' Hamiltonian H_{cl} note that

$$\begin{aligned}\sqrt{\alpha^{-2}q_j^2 + \alpha^{-4}} - \alpha^{-2} &= \alpha^{-2}\Big(\sqrt{1 + (\alpha q_j)^2} - 1\Big) \\ &\approx \alpha^{-2}\Big(1 + \frac{1}{2}(\alpha q_j)^2) - 1\Big) = \frac{q_j^2}{2}\end{aligned}$$

in the non-relativistic limit, that is, for αq_j small, so that

$$H_{cl} = R_\infty \left\{ \sum_{j=1}^{N} \left\{ \frac{q_j^2}{2} - \frac{Z}{|y_j|} \right\} + \sum_{1\le i<j\le N} \frac{1}{|y_i - y_j|} \right\}.$$

Since

$$\alpha^{-2}\Big(\sqrt{1 + (\alpha q_j)^2} - 1\Big) \le \frac{q_j^2}{2}$$

for all α and all q_j, one gets, that

$$\langle \psi, H_{rel}\psi\rangle \le \langle \psi, H_{cl}\psi\rangle$$

for all $\psi \in \mathcal{H}_F = \bigwedge^N L^2(\mathbb{R}^3, \mathbb{C}^2)$. In Thomas-Fermi theory, this immediately proves the upper bound on the relativistic quantum mechanical energy H_{rel} by the semi-classical Thomas-Fermi energy by Lieb and Simon's proof [12] of this bound on the 'classical' Hamiltonian H_{cl}; see also Lieb [9].

Appendix B. A formula for the kinetic energy

In this appendix we shall prove the localisation-formula (4.1) 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 [2, Theorem 3.2]). Let firstly K_2 be a modified Bessel-function of second order, defined on $(0, \infty)$ by

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

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:

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

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

Lemma B.1. *For $f \in \mathcal{S}(\mathbb{R}^3)$ with Fourier transform $\hat{f}$, one has*

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

Proof. Note, that by dominated convergence in momentum space, one has

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

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 [4]. In this way,

$$\begin{aligned}(f,&e^{-t\sqrt{p^2+\alpha^{-2}}}f)\\ &= \frac{t\alpha^{-2}}{2\pi^2}\iint \overline{f(x)}f(y)\frac{K_2\big[\alpha^{-1}(|x-y|^2+t^2)^{1/2}\big]}{|x-y|^2+t^2}\,d^3x\,d^3y. \end{aligned}\tag{B.3}$$

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

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

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

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

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

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

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

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

This proves the lemma. □

Now, to prove the formula (B.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 (B.2):

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

Using now, that

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

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

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

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

We now derive two facts about the function K_2:

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

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

The proof of (B.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

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

For the estimate (B.7), we need to rewrite K_2. This is done following Gray and Mathews [6, pp. 50].

Observation B.2.

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

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

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

Using the formula (to be found in any table of integrals)

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

with $a = \sqrt{t^2+\eta}$, $b = 1/2$, we arrive at

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

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

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

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

$$\begin{aligned}
K_2(t) &\le \sqrt{\frac{\pi}{2t}} \frac{1}{\Gamma(\frac{5}{2})} e^{-t} \int_0^\infty e^{-\xi}\xi^{3/2}\big(1 + \frac{3}{4t}\xi + \frac{3}{32t^2}\xi^2\big)\, d\xi \\
&= \sqrt{\frac{\pi}{2t}} \frac{1}{\Gamma(\frac{5}{2})} e^{-t} \Big(\int_0^\infty e^{-\xi}\xi^{3/2}\, d\xi \\
&\qquad\qquad + \frac{3}{4t}\int_0^\infty e^{-\xi}\xi^{5/2}\, d\xi + \frac{3}{32t^2}\int_0^\infty e^{-\xi}\xi^{7/2}\, d\xi \Big) \\
&= \sqrt{\frac{\pi}{2t}} \frac{1}{\Gamma(\frac{5}{2})} e^{-t} \Big(\Gamma(\tfrac{5}{2}) + \frac{3}{4t}\Gamma(\tfrac{7}{2}) + \frac{3}{32t^2}\Gamma(\tfrac{9}{2}) \Big) \\
&= \sqrt{\frac{\pi}{2t}} e^{-t}\big(1 + \frac{15}{8t} + \frac{105}{128t^2}\big) \le 4\sqrt{\frac{\pi}{2t}} e^{-t}\big(1 + \frac{1}{2t} + \frac{1}{(2t)^2}\big).
\end{aligned}$$

Appendix C. 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 C.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*

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

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):

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

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:

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

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 $\sqrt{p^2+\alpha^{-2}}$:

$$\begin{aligned}(f,\sqrt{p^2+\alpha^{-2}}f) &= \frac{1}{2}\iint \overline{f(x)}g(x-q)^2\big(\sqrt{p^2+\alpha^{-2}}f\big)(x)\,d^3q\,d^3x\\ &+\frac{1}{2}\iint \overline{\big(\sqrt{p^2+\alpha^{-2}}f\big)(x)}\,g(x-q)^2f(x)\,d^3q\,d^3x\\ &=\frac{1}{2}\iint \overline{f(x)}g_q(x)^2\big(\sqrt{p^2+\alpha^{-2}}f\big)(x)\,d^3q\,d^3x\\ &+\frac{1}{2}\iint \overline{f(x)}\Big(\sqrt{p^2+\alpha^{-2}}\big({g_q}^2f\big)\Big)(x)\,d^3q\,d^3x. \qquad (C.4)\end{aligned}$$

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

$$\begin{aligned}C.4 = \frac{1}{2}\iint &\overline{f(x)}\Big[\big({g_q}^2\sqrt{p^2+\alpha^{-2}}\\ &+\sqrt{p^2+\alpha^{-2}}{g_q}^2-2g_q\sqrt{p^2+\alpha^{-2}}g_q\big)f\Big](x)\,d^3q\,d^3x\\ +\iint &\overline{(g_qf)(x)}\big[\sqrt{p^2+\alpha^{-2}}(g_qf)\big](x)\,d^3q\,d^3x\\ =\frac{1}{2}\iint &\overline{f(x)}\big(L_qf\big)(x)\,d^3q\,d^3x\\ +\iint &\Big(\int\sqrt{p^2+\alpha^{-2}}\Big(\int e^{-ipy}g_q(y)f(y)\,d^3y\Big)e^{ipx}\,d^3p\Big)\\ &g_q(x)\overline{f(x)}\,d^3q\,d^3x \qquad (C.5)\end{aligned}$$

where

$$\begin{aligned}\big(L_qf\big)(x)=\int\Big\{\int &\big[g_q(y)^2+g_q(x)^2\\ &-2g_q(x)g_q(y)\big]\sqrt{p^2+\alpha^{-2}}e^{ip(x-y)}\,d^3p\Big\}f(y)\,d^3y.\end{aligned} \qquad (C.6)$$

The second term in (C.5) 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 (C.5) is the error, which will now be estimated. Keeping x and y fixed, we have, as showed in the proof of (B.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

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

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

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

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

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

□

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 $\mathrm{Vol}(\mathrm{supp}\ g_\alpha) = \frac{4\pi}{3}\alpha^{3s}$, and therefore

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

since, as $s < 2/3$,

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

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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