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by

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THE RELATIVISTIC SCOTT CORRECTION FOR ATOMS AND MOLECULES

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ABSTRACT. We prove the first correction to the leading Thomas-Fermi energy for the ground state energy of atoms and molecules in a model where the kinetic energy of the electrons is treated relativistically. The leading Thomas-Fermi energy, established in [25], as well as the correction given here are of semi-classical nature. Our result on atoms and molecules is proved from a general semi-classical estimate for relativistic operators with potentials with Coulomb-like singularities. This semi-classical estimate is obtained using the coherent state calculus introduced in [36]. The paper contains a unified treatment of the relativistic as well as the non-relativistic case.

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1. INTRODUCTION AND MAIN RESULTS

Our goal in this paper is to study how relativistic effects influence the energies of atoms and molecules. More specifically, we are aiming at proving a relativistic analog of the celebrated Scott correction [29, 16, 13, 15, 30, 31, 32, 36]. At present there is no mathematically well-defined fully relativistically invariant theory of atoms and molecules. We will here consider a simplified model, which shows the relevant qualitative features of relativistic effects. In this model, these effects are introduced by treating the kinetic energy of electrons of mass m by the operator $\sqrt{-\hbar^2\mathrm{c}^2\Delta + \mathrm{m}^2\mathrm{c}^4} - \mathrm{mc}^2$ instead of the standard non-relativistic Laplace operator $-\hbar^2\Delta/2\mathrm{m}$. Here c refers to the speed of light and $\hbar$ is Planck's constant. It is the simplest of a class of models that attempts to include relativistic effects; see [12, 23]. Although this model does not give accurate numerical agreement with observations it is from a qualitative point of view quite realistic.

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One of the qualitative features that our model shares with all other relativistic models is the instability of large atoms or molecules. The natural parameter to measure relativistic corrections in atoms and molecules is the dimensionless fine-structure constant $\alpha = \mathrm{e}^2/\hbar\mathrm{c}$, where e is the electron charge. As we will explain below, if $Z\alpha$ is too large (Z is the atomic number) then atoms are unstable. In our model the critical value of $Z\alpha$ is too small compared with experimental results and with what is assumed to be the correct critical value, namely $Z\alpha = 1$.

Our main interest here is the behavior of the total ground state energy of large atoms and molecules. Because of the relativistic instability problem mentioned above one cannot simply consider the limit of large atomic number Z. One is forced to look at the simultaneous limit of small fine-structure constant α in such a way that the product $Z\alpha$ remains bounded. Of course, α has a fixed value which experimentally is approximately $1/137$. Thus considering the limit α tending to zero is strictly speaking not physically correct. Likewise, considering the limit of Z tending to infinity is in contradiction with the fact that the experimentally observed values of Z are bounded (by 92 for the stable atoms). Studying the limit $Z \to \infty$ and $\alpha \to 0$ with $Z\alpha$ bounded allows us to make a precise mathematical statement about the asymptotics. There is numerical evidence that the asymptotics is indeed a good approximation to the total ground state energy for the physical values of Z and α.

The first to, at least heuristically, suggest to consider $Z\alpha$ as a separate parameter in the limit $Z \to \infty$ was Schwinger [27]. In this original paper, Schwinger finds discrepancies of his estimates of relativistic corrections with numerical evidence. Later [8], more corrections are taken into account and excellent agreement is found. This accuracy however goes beyond a rigorous mathematical treatment. We content ourselves with giving a rigorous treatment of the simplified model with the correct qualitative behavior.

The first rigorous treatment of the limit $Z \to \infty$ with $Z\alpha$ bounded was given by one of us is the paper [25], where the leading asymptotics of the ground state energy was found. It turns out it does not depend on $Z\alpha$. The goal of the present paper is the first correction to the leading asymptotics, i.e., the Scott correction and, in particular, to show that it depends on $Z\alpha$. The work in [25] was generalized to another relativistic model in [4].

We now introduce the molecular many-body Hamiltonian we consider in this paper. Let e and m denote the electric charge and mass of an electron. Let $\mathbf{Z}\mathrm{e} = (Z_1\mathrm{e}, \ldots, Z_M\mathrm{e})$, where $Z_1, \ldots, Z_M > 0$, be the charges of the M nuclei. We consider the Born-Oppenheimer formulation where these nuclei are at fixed positions $\mathbf{R} = (R_1, \ldots, R_M) \in \mathbb{R}^{3M}$. We have N electrons. As explained above the relativistic kinetic energy of the j-th electron is equal to $\sqrt{-\hbar^2\mathrm{c}^2\Delta_j + \mathrm{m}^2\mathrm{c}^4} - \mathrm{mc}^2$, where Δ_j is the Laplacian with respect to the j-th electron coordinate $y_j \in \mathbb{R}^3$, $j = 1, \ldots, N$. The potential energy of the electrons is composed of the attraction to the nuclei,

$$\mathrm{e}V(\mathbf{Z}\mathrm{e}, \mathbf{R}, y) = \sum_{k=1}^{M} \frac{Z_k \mathrm{e}^2}{|y - R_k|}\,, \tag{1}$$

and the electron-electron repulsion,

$$\sum_{1 \le i < j \le N} \frac{\mathrm{e}^2}{|y_i - y_j|}\,.$$

The total energy of the electrons is described by the Hamiltonian,

$$H_{\mathrm{rel}} = \sum_{j=1}^{N} \left[\sqrt{-\hbar^2\mathrm{c}^2\Delta_j + \mathrm{m}^2\mathrm{c}^4} - \mathrm{mc}^2 - \mathrm{e}V(\mathbf{Z}\mathrm{e}, \mathbf{R}, y_j)\right] + \sum_{1 \le i < j \le N} \frac{\mathrm{e}^2}{|y_i - y_j|}\,.$$

Let us now introduce the fundamental constants. Namely, let $a = \hbar^2/\mathrm{me}^2$ be the Bohr radius, and $R_\infty = \frac{1}{2}\mathrm{me}^4/\hbar^2$ Rydberg's constant. Then by a change of coordinates $y_j \to x_j = y_j/a$, we see that

$$\begin{aligned}(2R_\infty)^{-1}H_{\mathrm{rel}} &=: H(\mathbf{Z},\mathbf{R};\alpha) = H(Z_1,\ldots,Z_M,R_1,\ldots,R_M;\alpha)\\ &= \sum_{j=1}^{Z}\Big[\sqrt{-\alpha^{-2}\Delta_j+\alpha^{-4}}-\alpha^{-2}-V(\mathbf{Z},\mathbf{R},x_j)\Big]+\sum_{1\le i<j\le N}\frac{1}{|x_i-x_j|}\,,\end{aligned}$$

where again α is the fine-structure constant. For $\alpha = 0$ the kinetic energy of the j-th electron is $-\frac{1}{2}\Delta$.

Here we have set $N = Z = \sum_{k=1}^{M} Z_k$ so that the molecule is neutral. In particular, this means that Z must be an integer. From now on we study the operator $H(\mathbf{Z},\mathbf{R};\alpha)$. This operator acts as an unbounded operator on the anti-symmetric tensor product, $\bigwedge^Z L^2(\mathbb{R}^3 \times \{-1,1\})$, where ± 1 refers to the spin variables. We are interested in the ground state energy

$$E(\mathbf{Z},\mathbf{R};\alpha) = \inf\sigma\big(H(\mathbf{Z},\mathbf{R};\alpha)\big)\,,$$

and, in particular, in an asymptotic expansion of this when $Z \to \infty$.

The ground state energy $E(\mathbf{Z},\mathbf{R};\alpha)$ is finite if $\max_k\{Z_k\alpha\} \le 2/\pi$, but $E(\mathbf{Z},\mathbf{R};\alpha) = -\infty$ if $\max_k\{Z_k\alpha\} > 2/\pi$ (see [12, 23])[1]. This is the relativistic instability discussed above. Therefore we must require the atomic numbers to be smaller than or equal to $2/(\pi\alpha)$ which is approximately 87. This is of course in contradiction with the experimental fact that larger stable atoms exist and is one reason why our model can only be qualitatively correct. (We want to emphasise that the instability we are discussing here is not the nuclear instability causing atoms larger than atomic number 92 to be unstable. The relativistic instability we discuss here is only believed to manifest itself for atomic numbers greater than 137.)

The true energy of the molecule should include the nuclear-nuclear repulsion. Since the nuclei are considered fixed here the nuclear-nuclear repulsion is simply a constant which we have omitted.

As discussed above the leading asymptotics of $E(\mathbf{Z},\mathbf{R};\alpha)$ will be independent of the relativistic parameter α. It will be given by what is called Thomas-Fermi theory. The seminal contribution by Lieb and Simon [21] was to put Thomas-Fermi theory on a solid mathematical foundation and to prove that in the non-relativistic case the Thomas-Fermi energy of a molecule is indeed the correct leading asymptotic energy for the true ground state energy as $Z \to \infty$. This is the result that was generalized to our relativistic model in [25].

The main result of this paper is the following asymptotic result on the ground state energy.

Theorem 1 (Relativistic Scott correction). *Let $\mathbf{z} = (z_1,\ldots,z_M)$ with $z_1,\ldots,z_M > 0$, $\sum_{k=1}^M z_k = 1$, and $\mathbf{r} = (r_1,\ldots,r_M) \in \mathbb{R}^{3M}$ with $\min_{k\neq\ell}|r_k - r_\ell| > r_0$ for some $r_0 > 0$ be given. Define $\mathbf{Z} = (Z_1,\ldots,Z_M) = Z\mathbf{z}$ and $\mathbf{R} = Z^{-1/3}\mathbf{r}$. Then there exist a constant $E^{\mathrm{TF}}(\mathbf{z},\mathbf{r})$ and a universal (independent of $\mathbf{z}$, $\mathbf{r}$ and M) continuous, non-increasing function $\mathcal{S} : [0, 2/\pi] \to \mathbb{R}$ with $\mathcal{S}(0) = 1/4$ such that as $Z = \sum_{k=1}^M Z_k \to \infty$ and $\alpha \to 0$ with $\max_k\{Z_k\alpha\} \le 2/\pi$ we have*

$$E(\mathbf{Z},\mathbf{R};\alpha) = Z^{7/3}E^{\mathrm{TF}}(\mathbf{z},\mathbf{r}) + 2\sum_{k=1}^{M} Z_k^2\mathcal{S}(Z_k\alpha) + \mathcal{O}(Z^{2-1/30})\,. \tag{2}$$

[1]Here, and in the sequel, operators are defined as the Friedrichs extension for the corresponding form sum, originally defined on C_0^∞-functions (here, for instance, $\bigwedge^Z C_0^\infty(\mathbb{R}^3 \times \{-1,1\})$).

Here the error term means that $|\mathcal{O}(Z^{2-1/30})| \leq CZ^{2-1/30}$*, where the constant* C *only depends on* r_0 *and* M*. As before,* $\sqrt{-\alpha^{-2}\Delta+\alpha^{-4}}-\alpha^{-2} = -\frac{1}{2}\Delta$ *when* $\alpha = 0$*.*

Remark 2. A less detailed version of our result was announced in [35].

Remark 3. Several features of our result and its proof should be stressed:

(i) The constant $E^{\mathrm{TF}}(\mathbf{z},\mathbf{r})$ is determined in Thomas-Fermi theory.
(ii) The fact that $\mathbf{R} = Z^{-1/3}\mathbf{r}$ is the relevant scaling of the nuclear coordinates may, as we shall see, be understood from Thomas-Fermi theory.
(iii) A characterization of the function $\mathcal{S}$ is given explicitly in Corollary 6 below (see also Lemma 25). Its continuity is proved in Theorem 4.
(iv) The asymptotic result is uniform in the parameters $Z_k\alpha \in [0, 2/\pi]$, $k = 1,\ldots,M$.
(v) The result contains, as a special case, the non-relativistic situation $Z_k\alpha = 0$ and, in particular, the non-relativistic limit is controlled due to the continuity of the function $\mathcal{S}$ and the uniformity in the parameters $Z_k\alpha$. In order to get the non-relativistic limit it is important that all estimates have the correct non-relativistic behavior. This is an important issue in this work. Note that in the non-relativistic case the value $\mathcal{S}(0) = 1/4$ is explicitly known, whereas this is not the case for any other value. This is because the eigenvalues of Hydrogen are explicitly known in the non-relativistic case, but not in this relativistic case. The technique to prove a Scott-correction without knowing explicitly the eigenvalues for the one-body Hydrogen(like) operator was invented by Sobolev [33].
(vi) The proof of Theorem 1 does not rely on knowing the non-relativistic case, but treats both the relativistic and non-relativistic case simultaneously.
(vii) The situation near the critical value $Z_k\alpha = 2/\pi$ is understood since the function $\mathcal{S}$ is continuous up to the critical value $2/\pi$. This is, however, a less important point since we do not know whether the model we study gives a good description near the critical value.

The Scott correction was predicted by Scott [29] to be the first correction to the Thomas-Fermi energy. In the non-relativistic setting, this was mathematically established by Hughes [13], Siedentop and Weikard [30, 31, 32] for atoms (and by Bach [2] for ions) and later by Ivriĭ and Sigal [15] for molecules. Later a different proof was given by two of us for molecules [36]. Based on methods in [15], Balodis Matesanz [3] gave a proof for the Scott correction of matter. The Scott correction for operators with magnetic fields was studied by Sobolev [33, 34] (in the non-interacting case).

In [9], Fefferman and Seco derived rigorously the second correction to Thomas-Fermi theory for atoms, which is of the order $Z^{5/3}$. This was predicted by Dirac [7] and Schwinger [28]. It is apparently still an open problem to prove this for molecules and to find the relativistic correction to this order.

The main approach to proving the energy asymptotics for large atoms and molecules goes back to Lieb and Simon [21] and is to use semi-classical estimates. The Z-scaling makes it possible to relate the many-body problem to a one-body spectral problem, which may be treated semi-classically, where the semi-classical parameter is $h = Z^{-1/3}$. Here, several techniques have been developed. Lieb and Simon used Dirichlet–Neumann bracketing. This is however not refined enough to get beyond the leading term. The Weyl calculus [26] is the most advanced and precise method as far as optimal semi-classical error estimates are concerned, but it also will not directly give the Scott correction. Ivriĭ and Sigal [15] used Fourier intergral operator techniques to establish the non-relativistic Scott correction for molecules. Hughes and Siedentop–Weikard used methods that were designed particularly for spherically symmetric models, i.e., the atomic case.

A simple method, which is particularly well adapted to many-body problems is that of coherent states. It was pioneered by Lieb [16] and Thirring [37] to give very short proofs that Thomas-Fermi theory is correct to leading order. It is one of our major contributions here to use an improved calculus of coherent states as developed by two of us in [36] to the relativistic setting.

One feature of our work is that we give a general semi-classical estimate for relativistic one-body operators for potentials with singularities such as the Thomas-Fermi potential (see Theorem 4 below). This is derived by first proving a localised semi-classical estimate for potentials with some smoothness (see Theorem 32). The proof here is not much different from the one presented in [36] for non-relativistic Schrödinger operators. We do not claim that our error estimates are sharp given the regularity we assume on the potential, but only that they are sufficient to prove the Scott correction. In this connection we point out that in order to prove the Scott correction it is enough that the error relative to the leading term is smaller by more than one power of the semi-classical paramter h. In our case the relative error in Theorem 32 is $h^{6/5}$.

The relativistic kinetic energy is more cumbersome to work with than the Laplace operator and large parts of the rest of our proof from [36] have to be done differently. A main issue is to be able to localise into separate regions. Since the relativistic kinetic energy is a non-local operator, localisation estimates are more involved than in the non-relativistic setting. The philosophy is that localisation errors should behave as if we were working with non-relativistic local error terms up to some exponentially small tails (see Theorem 14).

The proof of the main theorem presented in Section 3 is based on the general semi-classical estimate Theorem 4 and the use of a correlation estimate (see Theorem 17) to reduce to the one-body problem.

After we had announced our results in [35], Frank, Siedentop, and Warzel [11] found a proof for the atomic case based on the method of Siedentop and Weikard [30, 31, 32], also [10] for the model studied in [4]. This approach seems to be restricted to the spherical case. This work does also not, contrary to the present work, make any special treatment of the non-relativistic limit or the continuity of the function $\mathcal{S}$.

1.1. **Main semi-classical result.** We consider the semi-classical approximation for the *relativistic* operator

$$T_\beta(-\mathrm{i}h\nabla) - V(\hat{x}),$$

where

$$T_\beta(p) = \begin{cases} \sqrt{\beta^{-1}p^2 + \beta^{-2}} - \beta^{-1}, & \beta \in (0,\infty) \\ \frac{1}{2}p^2, & \beta = 0 \end{cases}. \tag{3}$$

We will consider potentials $V : \mathbb{R}^3 \to \mathbb{R}$ with Coulomb singularities of the form $z_k|x-r_k|^{-1}$, $k = 1,\ldots,M$, at points $r_1,\ldots,r_M \in \mathbb{R}^3$ and with charges $0 < z_1,\ldots,z_M \leq 2/\pi$. Define

$$d_{\mathbf{r}}(x) = \min\left\{|x-r_k| \;\middle|\; k = 1,\ldots,M\right\}, \quad \mathbf{r} = (r_1,\ldots,r_M) \in \mathbb{R}^{3M}. \tag{4}$$

We assume that for some $\mu \geq 0$ the potential V satisfies

$$\left|\partial^\eta\big(V(x)+\mu\big)\right| \leq \begin{cases} C_{\eta,\mu} d_{\mathbf{r}}(x)^{-1-|\eta|} & \text{if } \mu \neq 0 \\ C_\eta \min\{d_{\mathbf{r}}(x)^{-1}, d_{\mathbf{r}}(x)^{-3}\}\, d_{\mathbf{r}}(x)^{-|\eta|} & \text{if } \mu = 0 \end{cases} \tag{5}$$

for all $x \in \mathbb{R}^3$ with $d_{\mathbf{r}}(x) \neq 0$ and all multi-indices η with $|\eta| \leq 3$, and

$$\big|V(x) - z_k|x - r_k|^{-1}\big| \leq C r_{\min}^{-1} + C \tag{6}$$

for $|x-r_k| < r_{\min}/2$ where $r_{\min} = \min_{k\neq\ell}|r_k - r_\ell|$. Note, in particular, that the Thomas-Fermi potential $V^{\mathrm{TF}}(\mathbf{z},\mathbf{r},\cdot)$ discussed in (35) below satisfies these requirements, by Theorem 20. So does the potential $V(x) = \frac{2}{\pi|x|} - 1$ (with $M = 1$, $r_0 = 0$, and $d_{\mathbf{r}}(x) = |x|$).

The main new result in this section is the relativistic Scott correction to the semi-classical expansion for potentials of this form. It will be proved in Section 4 below. The power -3 in (5) is not optimal.

Theorem 4 (**Scott-corrected relativistic semi-classics**). *There exists a continuous, non-increasing function $\mathcal{S} : [0, 2/\pi] \to \mathbb{R}$ with $\mathcal{S}(0) = 1/4$, such that for all $h > 0$, $0 \leq \beta \leq h^2$, T_β as in* (3)*, and all potentials $V : \mathbb{R}^3 \to \mathbb{R}$ satisfying* (5) *and* (6) *with $r_{\min} > r_0 > 0$ and $\max\{z_1, \ldots, z_M\} \leq 2/\pi$, we have*

$$\Big|\mathrm{Tr}\big[T_\beta(-\mathrm{i}h\nabla) - V(\hat{x})\big]_- - (2\pi h)^{-3}\int \big[\tfrac{1}{2}p^2 - V(v)\big]_-\,dvdp - h^{-2}\sum_{k=1}^{M} z_k^2\mathcal{S}(\beta^{1/2}h^{-1}z_k)\Big| \leq Ch^{-2+1/10}. \tag{7}$$

Here, $[x]_- = \min\{x, 0\}$. The constant $C > 0$ depends only on M, r_0, μ and the other constants in (5) *and* (6)*.*

Moreover, we can find a density matrix γ, whose density ρ_γ satisfies (with $\|\cdot\|_{6/5}$ the $L^{6/5}$-norm)

$$\Big|\int \rho_\gamma(x)\,dx - 2^{1/2}(3\pi^2)^{-1}h^{-3}\int |V(x)_-|^{3/2}\,dx\Big| \leq Ch^{-2+1/5} \tag{8}$$

and

$$\big\|\rho_\gamma - 2^{1/2}(3\pi^2)^{-1}h^{-3}|V_-|^{3/2}\big\|_{6/5} \leq Ch^{-2-1/10}, \tag{9}$$

such that

$$\mathrm{Tr}\big[(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x}))\gamma\big] \leq (2\pi h)^{-3}\int \big[\tfrac{1}{2}p^2 - V(v)\big]_-\,dvdp + h^{-2}\sum_{k=1}^{M} z_k^2\mathcal{S}(\beta^{1/2}h^{-1}z_k) + Ch^{-2+1/10}. \tag{10}$$

Remark 5. The term proportional to h^{-2} is called the *Scott correction.* If $\beta = h^2$ then it only depends on the charges $z_k, k = 1, \ldots, M$, of the Coulomb-singularities. Notice that the function in the semi-classical integral is the *non-relativistic* energy. This is also the reason why the leading Thomas-Fermi energy is independent of β.

Applying this theorem to the potential $V(x) = \frac{2}{\pi|x|} - 1$ (which satisfies (5) and (6) with $M = 1$, $r_0 = 0$, and $d_{\mathbf{r}}(x) = |x|$), and using a simple scaling argument, gives the following explicit characterization of the function $\mathcal{S}$ in Theorem 4 (see details in Lemma 27 in Section 4 below).

Corollary 6 (**Characterization of the Scott-correction $\mathcal{S}$**). *The function $\mathcal{S}$ satisfies, uniformly for $\alpha \in [0, 2/\pi]$,*

$$\mathcal{S}(\alpha) = \lim_{\kappa\to 0}\Big(\mathrm{Tr}\big[H_{\mathrm{C}} + \kappa\big]_- - (2\pi)^{-3}\int \big[\tfrac{1}{2}p^2 - |v|^{-1} + \kappa\big]_-\,dpdv\Big), \tag{11}$$

where

$$H_{\mathrm{C}}(\alpha) = \begin{cases} \sqrt{-\alpha^{-2}\Delta + \alpha^{-4}} - \alpha^{-2} - |\hat{x}|^{-1} \ , & \alpha \in (0, 2/\pi] \\ -\frac{1}{2}\Delta - |\hat{x}|^{-1} \ , & \alpha = 0 \end{cases} . \tag{12}$$

Remark 7. Another characterization of the function $\mathcal{S}$ is given in Lemma 25 in Section 4 below.

Remark 8. The result in Corollary 6 was proved in [24, Theorem 7.4], but only *pointwise* and only for $\alpha \in (0, 2/\pi)$.

2. Preliminaries

2.1. **Analytic tools.** We recall here the main analytic tools which we use throughout this paper. We do not prove all of them here but give the standard references. Various constants are denoted by the same letter C although its value may change from one line to the next.

Let $p \geq 1$, then a complex-valued function f (and only those will be considered here) is said to be in $L^p(\mathbb{R}^n)$ if the norm $\|f\|_p = \left(\int |f(x)|^p \, dx\right)^{1/p}$ is finite. We denote by $\langle \ , \ \rangle$ the inner product on $L^2(\mathbb{R}^n)$; it is linear in the second and anti-linear in the first entry. For any $1 \leq p \leq t \leq q \leq \infty$ we have the inclusion $L^p \cap L^q \subset L^t$, since by Hölder's inequality $\|f\|_t \leq \|f\|_p^{\lambda} \|f\|_q^{1-\lambda}$ with $\lambda p^{-1} + (1-\lambda) q^{-1} = t^{-1}$. We denote by $\hat{f}$ the Fourier transform of $f \in L^2(\mathbb{R}^n)$, given by $\hat{f}(p) = (2\pi)^{-n/2} \int \mathrm{e}^{-\mathrm{i}x \cdot p} f(x) \, dx$ for Schwartz functions on $\mathbb{R}^n$, and extended by continuity to $L^2(\mathbb{R}^n)$.

We denote $x_- = \min\{x, 0\}$, and let χ_A be the characteristic function of the set A; we write $\chi = \chi_{(-\infty,0]}$ for the characteristic function of $(-\infty, 0]$. We call γ a density matrix on $L^2(\mathbb{R}^n)$ if it is a trace class operator on $L^2(\mathbb{R}^n)$ satisfying the operator inequality $\mathbf{0} \leq \gamma \leq \mathbf{1}$. The density of a density matrix γ is the L^1-function ρ_γ such that $\mathrm{Tr}(\gamma\theta) = \int \rho_\gamma(x)\theta(x) dx$ for all $\theta \in C_0^\infty(\mathbb{R}^n)$ considered as a multiplication operator.

We also need an extension to many-particle states. Let $\psi \in \bigotimes^N L^2(\mathbb{R}^3 \times \{-1, 1\})$ be an N-body wave-function. Its one-particle density ρ_ψ is defined by

$$\rho_\psi(x) = \sum_{j=1}^{N} \sum_{s_1 = \pm 1} \cdots \sum_{s_N = \pm 1} \int |\psi(x_1, s_1, \ldots, x_N, s_N)|^2 \, \delta(x_j - x) \, dx_1 \cdots dx_N \, .$$

The following two inequalities we recall are crucial in many of our estimates. They serve as replacements for the Lieb-Thirring inequality [22] used in the non-relativistic case.

Theorem 9 (Daubechies inequality). One-body case: *Let $m > 0$, $f(u) = \sqrt{u^2 + m^2} - m$, and $F(s) = \int_0^s [f^{-1}(t)]^n \, dt$, where f^{-1} denotes the inverse function of f. Assume that $V \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$, and let $-\Delta$ be the Laplacian in $\mathbb{R}^n$. Then*

$$\mathrm{Tr}\big[\sqrt{-\Delta + m^2} - m + V(\hat{x})\big]_- \quad \geq \quad -C \int F\big(|V(x)_-|\big) \, dx \, , \tag{13}$$

where $x_- = \min\{x, 0\}$, and C is some positive constant.

Many-body case: *Let $\psi \in \bigwedge^N L^2(\mathbb{R}^3 \times \{-1, +1\})$ and let $\rho_\psi = \rho$ be its one-particle density. Then*

$$\Big\langle \psi, \sum_{j=1}^{N} \big[\sqrt{-\Delta_j + m^2} - m\big] \psi \Big\rangle \geq \int G[\rho(x)] \, dx \, , \tag{14}$$

where (with $C_0 = 0.326$)

$$G(\rho) = (3/8)m^4 C_0 g[(\rho/C_0)^{1/3}m^{-1}] - m\rho\,, \tag{15}$$

with $g(t) = t(1+t^2)^{1/2}(1+2t^2) - \log[t + (1+t^2)^{1/2}]$.

The asymptotic behaviour of G for small, respectively large ρ is given by

$$G(\rho) \underset{\rho\to 0}{\sim} (3/10m)C_0^{-2/3}\rho^{5/3}\,, \quad G(\rho) \underset{\rho\to\infty}{\sim} (3/4)C_0^{-1/3}\rho^{4/3}\,. \tag{16}$$

By a simple scaling, and using the definition of T and (16), respectively, we see that

$$\begin{aligned} &\mathrm{Tr}\big[\sqrt{-\alpha^{-2}\Delta + m^2\alpha^{-4}} - m\alpha^{-2} + V(\hat{x})\big]_- \\ &\quad \geq\; - Cm^{n/2}\int |V(x)_-|^{1+n/2}\,dx - C\alpha^n \int |V(x)_-|^{1+n}\,dx\,, \end{aligned} \tag{17}$$

and

$$\Big\langle \psi, \sum_{j=1}^N \big[\sqrt{-\alpha^{-2}\Delta_j + m^2\alpha^{-4}} - m\alpha^{-2}\big]\psi\Big\rangle \geq C\int \min\{m^{-1}\rho(x)^{5/3}, \alpha^{-1}\rho(x)^{4/3}\}\,dx\,. \tag{18}$$

Both (17) and (18) also holds for $\alpha = 0$, where we let $\sqrt{-\alpha^{-2}\Delta + m^2\alpha^{-4}} - m\alpha^{-2} = -\Delta/2m$, when $\alpha = 0$. The original proofs of the inequalities (13) and (14) can be found in [6] (for $\alpha = 0$, in [22]).

Theorem 10 (Lieb-Yau inequality). *Let $n = 3$. Let $C > 0$ and $R > 0$ and let*

$$H_{C,R} = \sqrt{-\Delta} - \frac{2}{\pi|\hat{x}|} - C/R\,. \tag{19}$$

Then, for any density matrix γ and any function θ with support in $B_R = \{x\,|\,|x| \leq R\}$ we have that

$$\mathrm{Tr}\big[\bar{\theta}\gamma\theta H_{C,R}\big] \geq -4.4827\,C^4 R^{-1}\{3/(4\pi R^3)\int |\theta(x)|^2\,dx\}\,. \tag{20}$$

Note that when $\theta = 1$ on B_R then the term inside the brackets $\{\}$ equals 1.

We will need the following new operator inequality. The proof can be found in Appendix A.

Theorem 11 (Critical Hydrogen inequality). *Let $n = 3$. For any $s \in [0, 1/2)$ there exists constants $A_s, B_s > 0$ such that*

$$\sqrt{-\Delta} - \frac{2}{\pi|\hat{x}|} \geq A_s(-\Delta)^s - B_s\,. \tag{21}$$

We also use the following standard notation for the Coulomb energy,

$$D(f) = D(f,f) = \tfrac{1}{2}\int \overline{f(x)}\,|x-y|^{-1} f(y)\,dxdy\,.$$

Theorem 12 (Hardy-Littlewood-Sobolev inequality). *There exists a constant C such that*

$$D(f) \leq C\,\|f\|_{6/5}^2\,. \tag{22}$$

The sharp constant C has been found by Lieb [18]; see also [19]. It can be shown by Fourier transformation that $f \mapsto \sqrt{D(f)}$ is a norm. This fact will play a role in the proof of the upper bound in our main Theorem 1.

In order to localise the relativistic kinetic energy we shall use the equivalent of the IMS-formula for the operator $-\Delta/2m$. In the sequel, as before, $\sqrt{-\alpha^{-2}\Delta + m^2\alpha^{-4}} - m\alpha^{-2} = -\Delta/2m$, when $\alpha = 0$.

Theorem 13 (**Relativistic IMS formula**). *Let $(\theta_u)_{u\in\mathcal{M}}$ be a family of positive bounded C^1-functions on $\mathbb{R}^3$ with bounded derivatives, and let $d\mu$ be a positive measure on $\mathcal{M}$ such that $\int_{\mathcal{M}} \theta_u(x)^2\, d\mu(u) = 1$ for all $x \in \mathbb{R}^3$. Then for any $f \in H^{1/2}(\mathbb{R}^3)$,*

$$\begin{aligned}&(f, (\sqrt{-\alpha^{-2}\Delta + m^2\alpha^{-4}} - m\alpha^{-2})f) \\ &\quad = \int_{\mathcal{M}} (\theta_u f, (\sqrt{-\alpha^{-2}\Delta + m^2\alpha^{-4}} - m\alpha^{-2})\theta_u f)\, d\mu(u) - (f, Lf)\,,\end{aligned} \tag{23}$$

where the operator L is of the form

$$L = \int_{\mathcal{M}} L_{\theta_u}\, d\mu(u)\,, \tag{24}$$

with L_{θ_u} the bounded operator with kernel

$$L_{\theta_u}(x,y) = (2\pi)^{-2} m^2 \alpha^{-3} |x-y|^{-2} K_2(m\alpha^{-1}|x-y|) \big[\theta_u(x) - \theta_u(y)\big]^2\,. \tag{25}$$

Here, K_2 is a modified Bessel function of the second kind. For $\alpha = 0$, L_{θ_u} is multiplication by $(\nabla\theta_u)^2/2m$, where $\sqrt{-\alpha^{-2}\Delta + m^2\alpha^{-4}} - m\alpha^{-2} = -\Delta/2m$, when $\alpha = 0$.

A proof (and the definition of K_2, and some of its properties) can be found in Appendix A. The following bound on the localisation error will be crucial.

Theorem 14 (**Localisation error**). *Let $\Omega \subset \mathbb{R}^3$ and $\ell > 0$. Let θ be a Lipschitz continuous function satisfying $0 \le \theta \le 1$, $\mathrm{dist}(\Omega^c, \mathrm{supp}\,\nabla\theta) \ge \ell$, and θ is constant on Ω^c.*

Then for all $m > 0$, $\alpha \ge 0$ there exists a positive operator Q_θ such that the following operator inequality holds:

$$L_\theta \le C\, m^{-1} \|\nabla\theta\|_\infty^2 \chi_\Omega + Q_\theta, \tag{26}$$

with

$$\mathrm{Tr}[Q_\theta] \le C\, m\alpha^{-2}\ell^{-1}\mathrm{e}^{-m\alpha^{-1}\ell}\|\nabla\theta\|_\infty^2 |\Omega|\,, \tag{27}$$

for a constant $C > 0$, independent of m, α, ℓ, θ, and Ω. Here, χ_Ω and $|\Omega|$ are the characteristic function and the volume, respectively, of the set Ω. For $\alpha = 0$, $Q_\theta \equiv 0$.

A proof can be found in Appendix A. Note that the first term, $C\, m^{-1}\|\nabla\theta\|_\infty^2\chi_\Omega$, on the right side of (26) is similar to the error in the non-relativistic IMS formula for the operator $-\Delta/2m$, except in this case one has $\|\nabla\theta\|_\infty^2 \chi_{\mathrm{supp}\nabla\theta}/2m$ as the only error.

When localising, we shall make use of the following.

Theorem 15 (**Partition of $\mathbb{R}^n$**). *Consider $\varphi \in C_0^\infty(\mathbb{R}^n)$ with support in the unit ball $\{|x| \le 1\}$ and satisfying $\int \varphi(x)^2\, dx = 1$. Assume that $\ell : \mathbb{R}^n \to \mathbb{R}$ is a C^1-map satisfying $0 < \ell(u) \le 1$ and $\|\nabla\ell\|_\infty < 1$. Let $J(x,u)$ be the Jacobian of the map $u \mapsto \frac{x-u}{\ell(u)}$, i.e.,*

$$J(x,u) = \ell(u)^{-n} \Big| \det\Big[\frac{(x_i - u_i)\partial_j \ell(u)}{\ell(u)} + \delta_{ij}\Big]_{ij} \Big|\,.$$

We set $\varphi_u(x) = \varphi\big(\frac{x-u}{\ell(u)}\big)\sqrt{J(x,u)}\,\ell(u)^{n/2}$. Then, for all $x \in \mathbb{R}^n$,

$$\int_{\mathbb{R}^n} \varphi_u(x)^2\, \ell(u)^{-n}\, du = 1\,, \tag{28}$$

and for all multi-indices $\eta \in \mathbb{N}^n$ we have

$$\|\partial^\eta \varphi_u\|_\infty \le \ell(u)^{-|\eta|} C_\eta \max_{|\nu|\le|\eta|} \|\partial^\nu\varphi\|_\infty\,, \tag{29}$$

where C_η depends only on η.

This is Theorem 22 in [36].

We will consider potentials $V : \mathbb{R}^3 \to \mathbb{R}$ with Coulomb singularities of the form $z_k|x - R_k|^{-1}$, $k = 1, \ldots, M$, at points $R_1, \ldots, R_M \in \mathbb{R}^3$ and with charges $0 < z_1, \ldots, z_M \le 2/\pi$. Recall that (see (4); replace $\mathbf{r}$ by $\mathbf{R}$)

$$d_{\mathbf{R}}(x) = \min\big\{|x - R_k| \;\big|\; k = 1, \ldots, M\big\}\ , \quad \mathbf{R} = (R_1, \ldots, R_M) \in \mathbb{R}^{3M}\,. \tag{30}$$

To treat such potentials we will need the following combination of Theorems 9 and 10. The proof can be found in Appendix A.

Theorem 16 (**Combined Daubechies-Lieb-Yau inequality**). *Let $R_1, \ldots, R_M \in \mathbb{R}^3$, and assume $W \in L^1_{\mathrm{loc}}(\mathbb{R}^3)$ satisfies*

$$W(x) \ge -\frac{\nu}{d_{\mathbf{R}}(x)} - C\nu m\alpha^{-1} \quad \text{when} \quad d_{\mathbf{R}}(x) < \alpha m^{-1}, \tag{31}$$

with $\alpha\nu \le 2/\pi$ and $m > 0$, $\alpha \ge 0$, and $d_{\mathbf{R}}$ as in (30)*. Assume also that the minimal distance between nuclei satisfies $\min_{k\neq\ell}|R_k - R_\ell| > 2\alpha m^{-1}$. Then*

$$\begin{aligned}&\mathrm{Tr}\big[\sqrt{-\alpha^{-2}\Delta + m^2\alpha^{-4}} - m\alpha^{-2} + W(\hat{x})\big]_-\\ &\ge\ -C\nu^{5/2}\alpha^{1/2}m - Cm^{3/2}\int\limits_{d_{\mathbf{R}}(x)>\alpha m^{-1}} |W(x)_-|^{5/2}\,dx - C\alpha^3\int\limits_{d_{\mathbf{R}}(x)>\alpha m^{-1}} |W(x)_-|^4\,dx\,,\end{aligned} \tag{32}$$

where as before $\sqrt{-\alpha^{-2}\Delta + m^2\alpha^{-4}} - m\alpha^{-2} = -\Delta/2m$, when $\alpha = 0$.

Finally, we come to the two inequalities which bound the many-body ground state energy in terms of a corresponding one-body energy.

Theorem 17 (**Correlation inequality**). *Let $\rho : \mathbb{R}^3 \to \mathbb{R}$ be non-negative with $D(\rho) < \infty$ and let $\Phi : \mathbb{R}^3 \to \mathbb{R}$ be a spherically symmetric, non-negative function with support in the unit ball such that $\int \Phi(x)\,dx < \infty$. For $s > 0$, let $\Phi_s(x) = s^{-3}\Phi(x/s)$. Then, for some constant C independent of N and s, we have*[2]

$$\sum_{1\le i<j\le N} |x_i - x_j|^{-1} \ge \sum_{j=1}^{N} (\rho * |x|^{-1} * \Phi_s)(x_j) - D(\rho) - CNs^{-1}\,. \tag{33}$$

The proof can be found in Appendix A.

Theorem 18 (**Lieb's Variational Principle**). *Let γ be a density matrix on $L^2(\mathbb{R}^3)$ satisfying $2\,\mathrm{Tr}\gamma = 2\int \rho_\gamma(x)\,dx \le Z$ (i.e., less than or equal to the total number of electrons) with kernel $\rho_\gamma(x) = \gamma(x,x)$. Then*

$$E(\mathbf{Z},\mathbf{R};\alpha) \le 2\,\mathrm{Tr}\big[\big(\sqrt{-\alpha^{-2}\Delta + \alpha^{-4}} - \alpha^{-2} - V(\mathbf{Z},\mathbf{R},\hat{x})\big)\gamma\big] + D(2\rho_\gamma)\,. \tag{34}$$

The factors 2 above are due to the spin degeneracy, see [17].

[2] We denote convolution by $*$, i.e., $(f*g)(x) = \int f(y)g(x-y)\,dy$. We also abuse notation and write $\rho*|x|^{-1}$ instead of $\big(\rho * |\cdot|^{-1}\big)(x)$.

2.2. **Thomas-Fermi theory.** Consider $\mathbf{z} = (z_1, \ldots, z_M) \in \mathbb{R}_+^M$ and $\mathbf{r} = (r_1, \ldots, r_M) \in \mathbb{R}^{3M}$. Let $0 \le \rho \in L^{5/3}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$ then the (non-relativistic) Thomas-Fermi (TF) energy functional, $\mathcal{E}^{\mathrm{TF}}$, is defined as

$$\mathcal{E}^{\mathrm{TF}}(\rho) = \tfrac{3}{10}(3\pi^2)^{2/3} \int \rho(x)^{5/3}\,dx - \int V(\mathbf{z}, \mathbf{r}, x)\rho(x)\,dx + D(\rho)\,,$$

where V is as in (1).

By the Hardy-Littlewood-Sobolev inequality the Coulomb energy, $D(\rho)$, is finite for functions $\rho \in L^{5/3}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3) \subset L^{6/5}(\mathbb{R}^3)$. Therefore, the TF-energy functional is well-defined. Here we only state without proof the properties about TF-theory which we use throughout the paper. The original proofs can be found in [21] and [16].

Theorem 19 (**Thomas-Fermi minimizer).** *For all $\mathbf{z} = (z_1, \ldots, z_M) \in \mathbb{R}_+^M$ and $\mathbf{r} = (r_1, \ldots, r_M) \in \mathbb{R}^{3M}$ there exists a unique non-negative $\rho^{\mathrm{TF}}(\mathbf{z}, \mathbf{r}, x)$ such that $\int \rho^{\mathrm{TF}}(\mathbf{z}, \mathbf{r}, x)\,dx = \sum_{k=1}^M z_k$ and*

$$\mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) = \inf\left\{\mathcal{E}^{\mathrm{TF}}(\rho) \;\middle|\; 0 \le \rho \in L^{5/3}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)\right\}.$$

We shall denote by $E^{\mathrm{TF}}(\mathbf{z}, \mathbf{r}) = \mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}})$ the TF-energy. Moreover, let

$$V^{\mathrm{TF}}(\mathbf{z}, \mathbf{r}, x) = V(\mathbf{z}, \mathbf{r}, x) - \rho^{\mathrm{TF}}(\mathbf{z}, \mathbf{r}, \cdot) * |x|^{-1} \tag{35}$$

be the TF-potential, then $V^{\mathrm{TF}} > 0$ and $\rho^{\mathrm{TF}} > 0$, and ρ^{TF} is the unique solution in $L^{5/3}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$ to the TF-equation:

$$V^{\mathrm{TF}}(\mathbf{z}, \mathbf{r}, x) = \tfrac{1}{2}(3\pi^2)^{2/3}\rho^{\mathrm{TF}}(\mathbf{z}, \mathbf{r}, x)^{2/3}\,. \tag{36}$$

Very crucial for a semi-classical approach is the *scaling* behavior of the TF-potential. It says that for any positive parameter h,

$$\begin{aligned} V^{\mathrm{TF}}(\mathbf{z}, \mathbf{r}, x) &= h^4 V^{\mathrm{TF}}(h^{-3}\mathbf{z}, h\mathbf{r}, hx)\,, && (37)\\ \rho^{\mathrm{TF}}(\mathbf{z}, \mathbf{r}, x) &= h^6 \rho^{\mathrm{TF}}(h^{-3}\mathbf{z}, h\mathbf{r}, hx)\,, && (38)\\ E^{\mathrm{TF}}(\mathbf{z}, \mathbf{r}) &= h^7 E^{\mathrm{TF}}(h^{-3}\mathbf{z}, h\mathbf{r})\,. && (39) \end{aligned}$$

By $h\mathbf{r}$ we mean that each coordinate is scaled by h, and likewise for $h^{-3}\mathbf{z}$ and hx. By the TF-equation (36), the equations (37) and (38) are obviously equivalent. Notice that the Coulomb-potential (the potential V in (1)) has the claimed scaling behavior. The rest follows from the uniqueness of the solution of the TF-energy functional.

We shall now establish the crucial estimates that we need about the TF-potential. For each $k = 1, \ldots, M$ we define the function

$$W_k(\mathbf{z}, \mathbf{r}, x) = V^{\mathrm{TF}}(\mathbf{z}, \mathbf{r}, x) - z_k|x - r_k|^{-1}\,. \tag{40}$$

The function W_k can be continuously extended to $x = r_k$.

The first estimate in the next theorem is very similar to a corresponding estimate in [15] (recall that the function $d_{\mathbf{r}}$ was defined in (4)).

Theorem 20 (**Estimate on V^{TF}).** *Let $\mathbf{z} = (z_1, \ldots, z_M) \in \mathbb{R}_+^M$ and $\mathbf{r} = (r_1, \ldots, r_M) \in \mathbb{R}^{3M}$. For all multi-indices $\eta \in \mathbb{N}^3$ and all x with $d_{\mathbf{r}}(x) \ne 0$ we have*

$$\left|\partial_x^\eta V^{\mathrm{TF}}(\mathbf{z}, \mathbf{r}, x)\right| \le C_\eta \min\{d_{\mathbf{r}}(x)^{-1}, d_{\mathbf{r}}(x)^{-4}\}\, d_{\mathbf{r}}(x)^{-|\eta|}\,, \tag{41}$$

where $C_\eta > 0$ is a constant which depends on η, $z_1, \ldots, z_M$, and M.

Moreover, for $|x - r_k| < r_{\min}/2$, where $r_{\min} = \min_{k \ne \ell}|r_k - r_\ell|$, we have

$$-C \le W_k(\mathbf{z}, \mathbf{r}, x) \le C r_{\min}^{-1} + C\,, \tag{42}$$

where the constants $C > 0$ here depend on $z_1, \dots, z_M$, and M.

Corollary 21 (**Estimate on $\rho^{\rm TF} * |x|^{-1} * (\delta_0 - \Phi_t)$**)**.** *Let $\Phi : \mathbb{R}^3 \to \mathbb{R}$ be a spherically symmetric, positive function with support in the unit ball and integral 1, and for $t > 0$, let $\Phi_t(x) = t^{-3}\Phi(x/t)$. If $\rho^{\rm TF}(x) = \rho^{\rm TF}(\mathbf{z}, \mathbf{r}, x)$ then*

$$0 \le \rho^{\rm TF} * |x|^{-1} - \rho^{\rm TF} * |x|^{-1} * \Phi_t \le \begin{cases} C\, t \min\{d_{\mathbf{r}}(x)^{-1/2}, d_{\mathbf{r}}(x)^{-2}\} & \text{for } d_{\mathbf{r}}(x) \ge 2t \\ C\, t^{1/2} & \text{for } d_{\mathbf{r}}(x) < 2t \end{cases} \tag{43}$$

with the function $d_{\mathbf{r}}$ from (4), and some constant $C > 0$ depending on $z_1, \dots, z_M$, and M.

For the proof of (41) and (42) we refer to [36]. (Note that in [36] it is claimed that $W_k(\mathbf{z}, \mathbf{r}, x) \ge 0$. This is not correct, but the proof in [36] does give that $W_k(\mathbf{z}, \mathbf{r}, x) \ge -C$.) The proof of (43) can be found in Appendix A.

Remark 22. As is seen from the proofs in [36] and in Appendix A, the constants in Theorem 20 and Corollary 21 only depend on $z_0 > 0$ when $z_1, \dots, z_M \in (0, z_0]$.

The relation of Thomas-Fermi theory to semi-classical analysis is that the semi-classical density of a gas of non-interacting (non-relativistic) electrons moving in the Thomas-Fermi potential $V^{\rm TF}$ is simply the Thomas-Fermi density. More precisely, the semi-classical approximation to the density of the projection onto the eigenspace corresponding to the negative eigenvalues of the Hamiltonian $-\frac{1}{2}\Delta - V^{\rm TF}$ is

$$2 \int_{\frac{1}{2}p^2 - V^{\rm TF}(\mathbf{z},\mathbf{r},x) \le 0} \frac{dp}{(2\pi)^3} = 2^{3/2}(3\pi^2)^{-1}(V^{\rm TF})^{3/2}(\mathbf{z}, \mathbf{r}, x) = \rho^{\rm TF}(\mathbf{z}, \mathbf{r}, x)\,. \tag{44}$$

Here the factor two on the very left is due to the spin degeneracy. Similarly, the semi-classical approximation to the energy of the gas, i.e., to the sum of the negative eigenvalues of $-\frac{1}{2}\Delta - V^{\rm TF}$, is

$$\begin{aligned} 2\int \big[\tfrac{1}{2}p^2 - V^{\rm TF}(\mathbf{z}, \mathbf{r}, x)\big]_- \frac{dx dp}{(2\pi)^3} &= -\tfrac{4\sqrt{2}}{15\pi^2} \int V^{\rm TF}(\mathbf{z}, \mathbf{r}, x)^{5/2}\, dx \\ &= E^{\rm TF}(\mathbf{z}, \mathbf{r}) + D\big(\rho^{\rm TF}(\mathbf{z}, \mathbf{r}, \cdot)\big)\,. \end{aligned} \tag{45}$$

Since (by Theorem 20) the Thomas-Fermi potential $V^{\rm TF}(\mathbf{z}, \mathbf{r}, \cdot)$ in (35) satisfies (5) and (6) (uniformly for $z_1, \dots, z_M \in (0, 2/\pi]$; see Remark 22), Theorem 4 implies that the density given in (44) and the energy given in (45) are the leading order terms also for the *relativistic* gas, i.e., for the operator $T_\beta(-ih\nabla) - V^{\rm TF}$, $0 \le \beta \le h^2$, with T_β as in (3). That the Thomas-Fermi energy is correct to leading order for $T_{h^2}(-ih\nabla) - V^{\rm TF}$ was proved in [25]. Theorem 4 establishes the first correction—the Scott correction—to the leading order.

3. Proof of the relativistic Scott correction for the molecular ground state energy

In this section we prove Theorem 1. Except for the correlation inequality we proceed in exactly the same manner as in the non-relativistic case [36]. In [36] correlations were controlled by the Lieb-Oxford inequality [20]. Applying this inequality, correlations can be estimated by the integral $\int \rho^{4/3}$ involving the electronic density ρ. Using the non-relativistic Lieb-Thirring inequality such an integral can be seen to be of lower order than the total energy. In the present relativistic case the Daubechies inequality (14) *a priori* only allows us to conclude that the integral $\int \rho^{4/3}$ is of the same order as the total energy. We therefore follow a different strategy.

Proof of Theorem 1 (**Lower bound**). Let ψ be a (normalised) ground state wave function and let $s>0$. We will use the correlation inequality (33) with $\rho(x)=\rho^{\rm TF}(\mathbf{Z},\mathbf{R},x)$. Let Φ_s be a function as in Theorem 17. We shall choose $s=Z^{-5/6}$.

As above (see (4)) we have $d_{\mathbf{r}}(x)=\min\{|x-r_k|\mid k=1,\ldots,M\}$. Note that for the physical positions of the nuclei we then have

$$d_{\mathbf{R}}(x)=\min\{|x-R_k|\mid k=1,\ldots,M\}=Z^{-1/3}d_{\mathbf{r}}(Z^{1/3}x)\,.$$

From the estimate in (43) with $t=Z^{1/3}s$ we obtain from the Thomas-Fermi scaling (38) that

$$\big|\rho^{\rm TF}(\mathbf{Z},\mathbf{R},\cdot)*|x|^{-1}-\rho^{\rm TF}(\mathbf{Z},\mathbf{R},\cdot)*|x|^{-1}*\Phi_s(x)\big|\leq CZ^{3/2}s(g(x)+Z^{1/6})\,,$$

where

$$g(x)=\begin{cases}(2s)^{-1/2} & \text{if } d_{\mathbf{R}}(x)<2s\\ d_{\mathbf{R}}(x)^{-1/2} & \text{if } 2s\leq d_{\mathbf{R}}(x)\leq Z^{-1/3}\\ 0 & \text{if } Z^{-1/3}<d_{\mathbf{R}}(x)\end{cases}.$$

We find from the correlation estimate (Theorem 17) that

$$\begin{aligned}
&\big\langle\psi,H(\mathbf{Z},\mathbf{R};\alpha)\psi\big\rangle\\
&\geq\ \sum_{j=1}^{Z}\big\langle\psi,\big[\sqrt{-\alpha^{-2}\Delta_j+\alpha^{-4}}-\alpha^{-2}-V(\mathbf{Z},\mathbf{R},\hat{x}_j)\big]\psi\big\rangle\\
&\quad+\big\langle\psi,\sum_{j=1}^{Z}\big(\rho^{\rm TF}(\mathbf{Z},\mathbf{R},\cdot)*|x|^{-1}*\Phi_s\big)(\hat{x}_j)\psi\big\rangle-D\big(\rho^{\rm TF}(\mathbf{Z},\mathbf{R},\cdot)\big)-Cs^{-1}Z\\
&\geq\ 2\,\mathrm{Tr}\big[\sqrt{-\alpha^{-2}\Delta+\alpha^{-4}}-\alpha^{-2}-V^{\rm TF}(\mathbf{Z},\mathbf{R},\hat{x})-CZ^{3/2}sg(\hat{x})\big]_{-}-D\big(\rho^{\rm TF}(\mathbf{Z},\mathbf{R},\cdot)\big)\\
&\quad-CsZ^{8/3}-Cs^{-1}Z\,.
\end{aligned}\tag{46}$$

To control the error term with g above we shall use the combined Daubechies-Lieb-Yau inequality (Theorem 16) to estimate

$$\varepsilon\,\mathrm{Tr}\big[\sqrt{-\alpha^{-2}\Delta+\alpha^{-4}}-\alpha^{-2}-V^{\rm TF}(\mathbf{Z},\mathbf{R},\hat{x})-C\varepsilon^{-1}Z^{3/2}sg(\hat{x})\big]_{-}$$

for some $0<\varepsilon<1$ which we will choose to be $\varepsilon=Z^{-1/2}$. We use Theorem 16 with $m=1$ and $\nu=\max_k Z_k$. Then by assumption $\nu\alpha\leq 2/\pi$. We must also check that the assumption (31) is satisfied, i.e., that for $d_{\mathbf{R}}(x)<\alpha$ we have

$$-V^{\rm TF}(\mathbf{Z},\mathbf{R},x)-C\varepsilon^{-1}Z^{3/2}sg(x)\geq-\frac{\nu}{d_{\mathbf{R}}(x)}-C\nu\alpha^{-1}\,.$$

This follows from the definition of g and the estimate on the TF potential in (42) together with the Thomas-Fermi scaling (37) if

$$\tfrac{1}{2}\alpha<s<C(\nu Z^{-1})^2(Z\alpha)^{-2}\varepsilon^2 Z,\qquad r_{\rm min}^{-1}+1<C(\nu Z^{-1})(Z\alpha)^{-1}Z^{2/3},$$

which, for Z large enough, is a consequence of the assumptions in the theorem and the choices of ε and s. Note, in particular, that $\nu Z^{-1}=\max_k z_k\geq M^{-1}$ (since $\sum_k z_k=1$) and by assumption $Z\alpha\leq\min_k 2/(\pi z_k)\leq 2M/\pi$. The constants C above depend only on $z_1,\ldots,z_M$, and M.

According to the Thomas-Fermi estimate (41), the Thomas-Fermi scaling (37), the definition of g, and the choices of s and ε we have

$$V^{\rm TF}(\mathbf{Z},\mathbf{R},x)+C\varepsilon^{-1}Z^{3/2}sg(x)\leq C\min\{d_{\mathbf{R}}(x)^{-4},Zd_{\mathbf{R}}(x)^{-1}\}\,.$$

Thus the combined Daubechies-Lieb-Yau inequality gives, since $\nu \le Z$ and $Z\alpha \le 2M/\pi$, that

$$\begin{aligned}
&\varepsilon \operatorname{Tr}\big[\sqrt{-\alpha^{-2}\Delta+\alpha^{-4}}-\alpha^{-2}-V^{\rm TF}(\mathbf{Z},\mathbf{R},\hat{x})-C\varepsilon^{-1}Z^{3/2}sg(\hat{x})\big]_-\\
\ge\ & -C\varepsilon Z^2-C\varepsilon\int\big(\min\{d_{\mathbf{R}}(x)^{-4},Zd_{\mathbf{R}}(x)^{-1}\}\big)^{5/2}dx\\
& -C\varepsilon\alpha^3\int_{d_{\mathbf{R}}(x)>\alpha}\big(\min\{d_{\mathbf{R}}(x)^{-4},Zd_{\mathbf{R}}(x)^{-1}\}\big)^{4}dx\\
\ge\ & -C\varepsilon(Z^2+Z^{7/3})\ge -C\varepsilon Z^{7/3}\,.
\end{aligned}$$

We return to the main term in (46). Using the Thomas-Fermi scaling property (37) and replacing x by $Z^{-1/3}x$ we arrive at

$$\begin{aligned}
&\operatorname{Tr}\big[\sqrt{-\alpha^{-2}\Delta+\alpha^{-4}}-\alpha^{-2}-V^{\rm TF}(\mathbf{Z},\mathbf{R},\hat{x})\big]_-\\
&\quad = \ Z^{4/3}\kappa^{-1}\operatorname{Tr}\big[\sqrt{-\beta^{-1}h^2\Delta+\beta^{-2}}-\beta^{-1}-\kappa V^{\rm TF}(\mathbf{z},\mathbf{r},\hat{x})\big]_-\,,
\end{aligned}$$

where we have chosen

$$\kappa=\min_k\frac{2}{\pi z_k}\ge Z\alpha\,,\qquad h=\kappa^{1/2}Z^{-1/3}\,,\qquad \beta=Z^{4/3}\alpha^2\kappa^{-1}\,. \tag{47}$$

We shall use β and h as the semi-classical parameters when we apply Theorem 4. It is therefore important that $\beta\le h^2$. This follows since $\beta^{-1}h^2=(Z\alpha)^{-2}\kappa^2\ge 1$. Note also that $2/\pi\le\kappa\le 2M/\pi$ since $z_k\le 1$, $k=1,\dots,M$, and $\sum_k z_k=1$.

Putting this together with the estimate above into (46) we obtain (using the inequality $\operatorname{Tr}[X+Y]_-\ge\operatorname{Tr}[X]_-+\operatorname{Tr}[Y]_-$ for operators X and Y bounded from below (with a common core), and the choices of ε and s) that

$$\begin{aligned}
&\big\langle\psi,H(\mathbf{Z},\mathbf{R};\alpha)\psi\big\rangle\\
&\ge\ 2(1-\varepsilon)Z^{4/3}\kappa^{-1}\operatorname{Tr}\big[\sqrt{-\beta^{-1}h^2\Delta+\beta^{-2}}-\beta^{-1}-\kappa V^{\rm TF}(\mathbf{z},\mathbf{r},\hat{x})\big]_-\\
&\quad -C\varepsilon Z^{7/3}-CsZ^{8/3}-Cs^{-1}Z-D\big(\rho^{\rm TF}(\mathbf{Z},\mathbf{R},\cdot)\big)\\
&\ge\ 2Z^{4/3}\kappa^{-1}\operatorname{Tr}\big[\sqrt{-\beta^{-1}h^2\Delta+\beta^{-2}}-\beta^{-1}-\kappa V^{\rm TF}(\mathbf{z},\mathbf{r},\hat{x})\big]_-\\
&\quad -D\big(\rho^{\rm TF}(\mathbf{Z},\mathbf{R},\cdot)\big)-CZ^{2-1/6}\,.
\end{aligned}$$

Now we apply the semi-classical result for potentials with Coulomb-like singularities from Theorem 4 to $\kappa V^{\rm TF}(\mathbf{z},\mathbf{r},\cdot)$ (recall that $2/\pi\le\kappa\le 2M/\pi$ which ensures that the constants in (5) and (6) are uniform in κ), and the calculation in (45). Then

$$\begin{aligned}
&2Z^{4/3}\kappa^{-1}\operatorname{Tr}\big[\sqrt{-\beta^{-1}h^2\Delta+\beta^{-2}}-\beta^{-1}-\kappa V^{\rm TF}(\mathbf{z},\mathbf{r},\hat{x})\big]_-\\
&=\ Z^{7/3}\Big(E^{\rm TF}(\mathbf{z},\mathbf{r})+D\big(\rho^{\rm TF}(\mathbf{z},\mathbf{r},\cdot)\big)\Big)+2\sum_{k=1}^M Z_k^2\mathcal{S}(Z_k\alpha)+\mathcal{O}(Z^{2-1/30})\\
&=\ E^{\rm TF}(\mathbf{Z},\mathbf{R})+D\big(\rho^{\rm TF}(\mathbf{Z},\mathbf{R},\cdot)\big)+2\sum_{k=1}^M Z_k^2\mathcal{S}(Z_k\alpha)+\mathcal{O}(Z^{2-1/30})\,.
\end{aligned}$$

Note here that κ cancels in the leading semi-classical term and in the Scott-term (the term with $\mathcal{S}$). Also, $2/\pi\le\kappa\le 2M/\pi$ ensures that the error is uniform in κ. Here we have again used the TF scaling $E^{\rm TF}(\mathbf{Z},\mathbf{R})=Z^{7/3}E^{\rm TF}(\mathbf{z},\mathbf{r})$ and $D\big(\rho^{\rm TF}(\mathbf{Z},\mathbf{R},\cdot)\big)=Z^{7/3}D\big(\rho^{\rm TF}(\mathbf{z},\mathbf{r},\cdot)\big)$. This finishes the proof of the lower bound. □

Proof of Theorem 1 (**Upper bound**). The starting point now is Lieb's variational principle, Theorem 18. By a simple rescaling the variational principle states that for any density matrix γ on $L^2(\mathbb{R}^3)$ with $2\,\mathrm{Tr}\gamma \le Z$ we have

$$\begin{aligned} E(\mathbf{Z},\mathbf{R};\alpha) \;&\le\; 2Z^{4/3}\,\mathrm{Tr}\big[\big(\sqrt{-\alpha^{-2}Z^{-2}\Delta+\alpha^{-4}Z^{-8/3}}-\alpha^{-2}Z^{-4/3}-V(\mathbf{z},\mathbf{r},\hat{x})\big)\gamma\big] \\ &\quad + Z^{7/3}D(2Z^{-1}\rho_\gamma)\,. \end{aligned}$$

As for the lower bound we bring the TF-potential into play:

$$\begin{aligned} Z^{-4/3}E(\mathbf{Z},\mathbf{R};\alpha) \;&\le\; 2\,\mathrm{Tr}\big[\big(\sqrt{-\alpha^{-2}Z^{-2}\Delta+\alpha^{-4}Z^{-8/3}}-\alpha^{-2}Z^{-4/3}-V^{\mathrm{TF}}(\mathbf{z},\mathbf{r},\hat{x})\big)\gamma\big] \\ &\quad + ZD\big(2Z^{-1}\rho_\gamma-\rho^{\mathrm{TF}}(\mathbf{z},\mathbf{r},\cdot)\big)-ZD\big(\rho^{\mathrm{TF}}(\mathbf{z},\mathbf{r},\cdot)\big) \\ &= 2\kappa^{-1}\,\mathrm{Tr}\big[\big(\sqrt{-\beta^{-1}h^2\Delta+\beta^{-2}}-\beta^{-1}-\kappa V^{\mathrm{TF}}(\mathbf{z},\mathbf{r},\hat{x})\big)\gamma\big] \\ &\quad + ZD\big(2Z^{-1}\rho_\gamma-\rho^{\mathrm{TF}}(\mathbf{z},\mathbf{r},\cdot)\big)-ZD\big(\rho^{\mathrm{TF}}(\mathbf{z},\mathbf{r},\cdot)\big)\,, \end{aligned} \tag{48}$$

where κ, h, and β are chosen as in (47) in the proof of the lower bound. Note that with this choice of h and κ we have from (36) that

$$2^{1/2}(3\pi^2h^3)^{-1}(\kappa V^{\mathrm{TF}}(\mathbf{z},\mathbf{r},x))^{3/2}=Z\rho^{\mathrm{TF}}(\mathbf{z},\mathbf{r},x)/2\,.$$

We now choose a density matrix $\widetilde{\gamma}$ according to Theorem 4 with $V(x)=\kappa V^{\mathrm{TF}}(\mathbf{z},\mathbf{r},x)$.

Since $\int\rho^{\mathrm{TF}}(\mathbf{z},\mathbf{r},x)\,dx=\sum_{k=1}^M z_k=1$ we see from (8) that $2\,\mathrm{Tr}\widetilde{\gamma}\le Z(1+CZ^{-1/3-1/15})$ (recall that $\kappa^{-1}\le\pi/2$). Thus if we define $\gamma=(1+CZ^{-1/3-1/15})^{-1}\widetilde{\gamma}$ we see that the condition $2\,\mathrm{Tr}\gamma\le Z$ is satisfied.

Using the Hardy-Littlewood-Sobolev and (9) inequalities we find that

$$ZD\big(2Z^{-1}\rho_{\widetilde{\gamma}}-\rho^{\mathrm{TF}}(\mathbf{z},\mathbf{r},\cdot)\big)\le CZ^{-1}\big\|\rho_{\widetilde{\gamma}}-Z\rho^{\mathrm{TF}}(\mathbf{z},\mathbf{r},\cdot)/2\big\|_{6/5}^2\le CZ^{2/3-4/15}\,,$$

and thus

$$\begin{aligned} ZD\big(2Z^{-1}\rho_\gamma-\rho^{\mathrm{TF}}(\mathbf{z},\mathbf{r},\cdot)\big) \;&\le\; C(1+CZ^{-1/3-1/15})^{-2}ZD\big(2Z^{-1}\rho_{\widetilde{\gamma}}-\rho^{\mathrm{TF}}(\mathbf{z},\mathbf{r},\cdot)\big) \\ &\quad + CZ^{1/3-2/15}D\big(\rho^{\mathrm{TF}}(\mathbf{z},\mathbf{r},\cdot)\big)\le CZ^{2/3-4/15}\,, \end{aligned} \tag{49}$$

where we have used the triangle inequality for $\sqrt{D}$, and that $D\big(\rho^{\mathrm{TF}}(\mathbf{z},\mathbf{r},\cdot)\big)\le C$.

Finally, if we use (10) and (45) we get as for the lower bound that

$$\begin{aligned} &2Z^{4/3}\kappa^{-1}\,\mathrm{Tr}\big[\big(\sqrt{-\beta^{-1}h^2\Delta+\beta^{-2}}-\beta^{-1}-\kappa V^{\mathrm{TF}}(\mathbf{z},\mathbf{r},\hat{x})\big)\widetilde{\gamma}\big] \\ &\le\; E^{\mathrm{TF}}(\mathbf{Z},\mathbf{R})+D\big(\rho^{\mathrm{TF}}(\mathbf{Z},\mathbf{R},\cdot)\big)+2\sum_{j=1}^M Z_k^2\mathcal{S}(Z_k\alpha)+\mathcal{O}(Z^{2-1/30})\,. \end{aligned}$$

Since $E^{\mathrm{TF}}(\mathbf{Z},\mathbf{R})\ge -CZ^{7/3}$ and $D\big(\rho^{\mathrm{TF}}(\mathbf{Z},\mathbf{R},\cdot)\big)\ge 0$ we see that the same estimate holds for $\widetilde{\gamma}$ replaced by γ. This together with $D\big(\rho^{\mathrm{TF}}(\mathbf{Z},\mathbf{R},\cdot)\big)=Z^{7/3}D\big(\rho^{\mathrm{TF}}(\mathbf{z},\mathbf{r},\cdot)\big)$, (48), and (49) finishes the proof of the upper bound. □

The function $\mathcal{S}$ is continuous and non-increasing, and $\mathcal{S}(0)=1/4$, according to Theorem 4. This finishes the proof of Theorem 1.

4. Relativistic semi-classics for potentials with Coulomb-like singularities

In this section we prove Theorem 4. The theorem will follow from using Theorem 23 below (a rescaled version of the local semi-classical results for *regular* potentials in Theorem 32 in Section 5 below). We localise (Theorem 13) the operator using multi-scale analysis (Theorem 15), and control the localisation errors (Theorem 16). Near the singularities of the potential, we compare with the Coulomb potential. To be able to do this, we first prove a Scott-corrected semi-classical result for a localised relativistic Hydrogen operator (Lemma 25 below). The ingredients of the proof of the latter are the same (rescaled semi-classics, localisation and multi-scale analysis, and estimating localisation errors).

Theorem 23 (**Rescaled semi-classics**). *Let $n \geq 3$ and let $\phi \in C_0^{n+4}(\mathbb{R}^n)$ be supported in a ball B_ℓ of radius $\ell > 0$. Let $V \in C^3(\overline{B_\ell})$ be a real potential, and let $T_\beta(p) = \sqrt{\beta^{-1}p^2 + \beta^{-2}} - \beta^{-1}$ be the kinetic energy. Let $H_\beta = T_\beta(-\mathrm{i}h\nabla) + V(\hat{x})$, $h > 0$, and $\sigma_\beta(v,q) = T_\beta(q) + V(v)$. Then for all $h, \beta, f > 0$ with $\beta f^2 \leq 1$, we have*

$$\left| \mathrm{Tr}[\phi H_\beta \phi]_- - (2\pi h)^{-n} \int \phi(v)^2 \sigma_\beta(v,q)_- \, dvdq \right| \leq C h^{-n+6/5} f^{n+4/5} \ell^{n-6/5}\,, \tag{50}$$

where the constant C is independent of β and depends only on

$$\sup_{|\eta| \leq n+4} \|\ell^{|\eta|}\partial^\eta \phi\|_\infty \quad \textit{and} \quad \sup_{|\eta|\leq 3} \|f^{-2}\ell^{|\eta|}\partial^\eta V\|_\infty\,. \tag{51}$$

Moreover, there exists a density matrix γ such that

$$\mathrm{Tr}[\gamma\phi H_\beta \phi] \leq (2\pi h)^{-n} \int \phi(v)^2 \sigma_\beta(v,q)_- \, dvdq + C h^{-n+6/5} f^{n+4/5} \ell^{n-6/5}\,. \tag{52}$$

The density ρ_γ satisfies

$$\left| \rho_\gamma(x) - (2\pi h)^{-n}\omega_n |V_-|^{n/2}(2 + \beta|V_-|)^{n/2}(x) \right| \leq C h^{-n+9/10} f^{n-9/10} \ell^{-9/10} \tag{53}$$

for (almost) all $x \in B_\ell$, and

$$\begin{aligned} &\left| \int \phi(x)^2 \rho_\gamma(x)\, dx - (2\pi h)^{-n}\omega_n \int \phi(x)^2 |V_-|^{n/2}(2+\beta|V_-|)^{n/2}(x)\, dx \right| \\ &\leq \; C h^{-n+6/5} f^{n-6/5} \ell^{n-6/5}\,, \end{aligned} \tag{54}$$

where ω_n is the volume of the unit ball B_1 in $\mathbb{R}^n$. The constants $C > 0$ in the above estimates again depend on the parameters as in (51).

Proof. We introduce the unitary scaling operator $(U\psi)(x) = \ell^{-n/2}\psi(\ell^{-1}x)$. Then

$$U^*\phi\big[T_\beta(-\mathrm{i}h\nabla) + V(\hat{x})\big]\phi\, U = f^2 \phi_\ell \big[T_{\beta f^2}(-\mathrm{i}hf^{-1}\ell^{-1}\nabla) + V_{f,\ell}(\hat{x})\big]\phi_\ell\,,$$

where $\phi_\ell(x) = \phi(\ell x)$, and $V_{f,\ell}(x) = f^{-2}V(\ell x)$. Thus,

$$\mathrm{Tr}[\phi H_\beta \phi]_- = f^2\, \mathrm{Tr}\Big[\phi_\ell\big[T_{\beta f^2}(-\mathrm{i}hf^{-1}\ell^{-1}\nabla) + V_{f,\ell}(\hat{x})\big]\phi_\ell\Big]_-\,.$$

Note that ϕ_ℓ and $V_{f,\ell}$ are supported in a ball of radius 1 and that for all multi-indices η,

$$\|\partial^\eta \phi_\ell\|_\infty = \|\ell^{|\eta|}\partial^\eta\phi\|_\infty \quad \text{and} \quad \|\partial^\eta V_{f,\ell}\|_\infty = f^{-2}\|\ell^{|\eta|}\partial^\eta V\|_\infty\,.$$

Let $\sigma_{f,\ell,\beta}(u,q) = T_{\beta f^2}(q) + V_{f,\ell}(u)$. By Theorem 32 in Section 5 below there is a constant C depending on the parameters as in (51) so that, as long as $\beta f^2 \leq 1$,

$$\left| \mathrm{Tr}[\phi H_\beta \phi]_- - (2\pi h f^{-1}\ell^{-1})^{-n} f^2 \int \phi_\ell(u)^2 \sigma_{f,\ell,\beta}(u,q)_-\, dudq \right| \leq C f^2 (hf^{-1}\ell^{-1})^{-n+6/5}\,. \tag{55}$$

A simple change of variables gives

$$(2\pi h f^{-1}\ell^{-1})^{-n} f^2 \int \phi_\ell(u)^2 \sigma_{f,\ell,\beta}(u,q)_-\, dudq = (2\pi h)^{-n} \int \phi(v)^2 \sigma_\beta(v,q)_-\, dvdq\,,$$

and we have proved (50).

Now, let $\gamma_{f,\ell,\beta}$ be the density matrix for $\phi_\ell\big[T_{\beta f^2}(-\mathrm{i}hf^{-1}\ell^{-1}\nabla)+V_{f,\ell}(\hat{x})\big]\phi_\ell$, which according to Lemma 34 satisfies

$$\begin{aligned}
&f^2\,\mathrm{Tr}\Big[\phi_\ell\big[T_{\beta f^2}(-\mathrm{i}hf^{-1}\ell^{-1}\nabla)+V_{f,\ell}(\hat{x})\big]\phi_\ell\gamma_{f,\ell,\beta}\Big]\\
&\quad\le\;(2\pi hf^{-1}\ell^{-1})^{-n}f^2\int\phi_\ell(u)^2\sigma_{f,\ell,\beta}(u,q)_-\,dudq+C(hf^{-1}\ell^{-1})^{-n+6/5}\,,
\end{aligned}$$

$$\begin{aligned}
&\Big|\rho_{\gamma_{f,\ell,\beta}}(x)-(2\pi hf^{-1}\ell^{-1})^{-n}\omega_n|V_{f,\ell}(x)_-|^{n/2}(2+\beta f^2|V_{f,\ell}(x)_-|)^{n/2}(x)\Big|\\
&\quad\le\;C(hf^{-1}\ell^{-1})^{-n+9/10}\,,
\end{aligned}$$

$$\begin{aligned}
&\Big|\int\phi_\ell(x)^2\rho_{\gamma_{f,\ell,\beta}}(x)\,dx-(2\pi hf^{-1}\ell^{-1})^{-n}\omega_n\int\phi_\ell(x)^2|V_{f,\ell}(x)_-|^{n/2}(2+\beta f^2|V_{f,\ell}(x)_-|)^{n/2}\,dx\Big|\\
&\le\;C(hf^{-1}\ell^{-1})^{-n+6/5}\,.
\end{aligned}$$

The density matrix $\gamma=U\gamma_{f,\ell,\beta}U^*$, whose density is $\rho_\gamma(x)=\ell^{-n}\rho_{\gamma_{f,\ell,\beta}}(x/\ell)$, then satisfies the properties in (52)–(54). $\square$

Multi-scale Analysis. The rescaled semi-classics of Theorem 23 will be used in balls of varying radius. This idea goes back to Ivriĭ [15, 14]. We introduce a variable scale ℓ and a corresponding family of localisation functions $\{\varphi_u\}_{u\in\mathbb{R}^3}$, which will also be used in the proof of Theorem 4.

Definition 24 (**Scale for multi-scale analysis).** *Let $0<\ell_0<1$ be a parameter that we shall choose explicitly below, and let $r_1,\ldots,r_M\in\mathbb{R}^3$. Define*

$$\ell(x)=\tfrac12\Big(1+\sum_{k=1}^{M}(|x-r_k|^2+\ell_0^2)^{-1/2}\Big)^{-1}\,. \tag{56}$$

Note that ℓ is a smooth function (due to ℓ_0) with

$$0<\ell(x)<1/2\quad\text{and}\quad\|\nabla\ell\|_\infty<1/2\,. \tag{57}$$

Note also that in terms of the function $d\equiv d_{\mathbf{r}}$ from (4) we have

$$\tfrac12(1+M)^{-1}\ell_0\le\tfrac12(1+M(d(x)^2+\ell_0^2)^{-1/2})^{-1}\le\ell(x)\le\tfrac12(d(x)^2+\ell_0^2)^{1/2}\,. \tag{58}$$

In particular, we have

$$\ell(x)\ge\tfrac12(1+M)^{-1}\min\{d(x),1\}\,. \tag{59}$$

We fix a localisation function $\varphi\in C_0^\infty(\mathbb{R}^3)$ with support in $\{|x|<1\}$ and such that $\int\varphi(x)^2\,dx=1$. According to Theorem 15 we can find a corresponding family of functions $\varphi_u\in C_0^\infty(\mathbb{R}^3)$, $u\in\mathbb{R}^3$, where φ_u is supported in the ball $\{|x-u|<\ell(u)\}$, with the properties that

$$\int_{\mathbb{R}^3}\varphi_u(x)^2\ell(u)^{-3}\,du\,=\,1\quad\text{and}\quad\|\partial^\eta\varphi_u\|_\infty\,\le\,C\ell(u)^{-|\eta|}\,, \tag{60}$$

for all multi-indices η, where $C>0$ depends only on η and φ. For $d(u)>2\ell_0$ we have $\ell(u)\le\sqrt5 d(u)/4$ and hence for all x with $|x-u|<\ell(u)$ we have (note that $d(u)\le d(x)+|x-u|$ and $\sqrt5/4<1$) that

$$\ell(u)<d(u)\quad\text{and}\quad d(u)\le Cd(x)\,. \tag{61}$$

As a first step towards the Scott correction for Coulomb-type potentials we deal with the Scott correction for a single relativistic Hydrogen atom. This method for proving the existence of a Scott correction in the semi-classical expansion of the sum of eigenvalues of an operator with a (homogeneous) singular potential without explicitly knowing the eigenvalues was first used by Sobolev [33] when studying (non-relativistic) operators with magnetic fields.

Lemma 25 (**Scott-corrected localised Hydrogen**). *There exists a non-increasing function $\mathcal{S} : [0, 2/\pi] \to \mathbb{R}$, with $\mathcal{S}(0) = 1/4$, such that, if $\phi_r(x) = \phi(x/r)$, $r \in (0,\infty)$, with $\phi \in C^7(\mathbb{R}^3)$, $0 \le \phi \le 1$, satisfying $\sqrt{1-\phi} \in C^1(\mathbb{R})$ and*

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

then there exists $C > 0$ depending only on ϕ such that for all $\alpha \in [0, 2/\pi]$ and $r \in (0,\infty)$,

$$\Big|\mathrm{Tr}[\phi_r H_{\mathrm{C}}(\alpha)\phi_r]_- - (2\pi)^{-3}\int \phi_r(v)^2\big[\tfrac12 q^2 - |v|^{-1}\big]_-\,dvdq - \mathcal{S}(\alpha)\Big| < Cr^{-1/10}\,, \tag{62}$$

where

$$H_{\mathrm{C}}(\alpha) = \begin{cases} \sqrt{-\alpha^{-2}\Delta + \alpha^{-4}} - \alpha^{-2} - |\hat{x}|^{-1}\,, & \alpha \in (0, 2/\pi] \\ -\tfrac12\Delta - |\hat{x}|^{-1}\,, & \alpha = 0 \end{cases}. \tag{63}$$

As emphasised in Remark 5, the function in the semi-classical integral in (62) is the *non-relativistic* energy. See also Lemma 27 below for an alternative description of the function $\mathcal{S}$.

Remark 26. A result similar to the one in Lemma 25 was proved in [24, Theorem 7.1], but without uniform control in α and only for $\alpha \in (0, 2/\pi)$.

Proof of Lemma 25. We fix $\alpha \in [0, 2/\pi]$ and write $H_{\mathrm{C}} = H_{\mathrm{C}}(\alpha)$. We define for $r > 0$

$$S_r = \mathrm{Tr}\big[\phi_r H_{\mathrm{C}}(\alpha)\phi_r\big]_- - (2\pi)^{-3}\int \phi_r(v)^2\big[\tfrac12 q^2 - |v|^{-1}\big]_-\,dvdq\,. \tag{64}$$

We will show that S_r has a limit as $r \to \infty$.

Let $R > 2r$. We estimate the difference between $\mathrm{Tr}[\phi_R H_{\mathrm{C}}\phi_R]_-$ and $\mathrm{Tr}[\phi_r H_{\mathrm{C}}\phi_r]_-$ semi-classically. The leading semi-classical term involves the relativistic energy which is then compared to the non-relativistic energy. Below all constants will depend only on ϕ and in particular *not* on $\alpha \in [0, 2/\pi]$.

Denote $\psi_r = \sqrt{1-\phi_r^2}$. By the relativistic IMS formula (23),

$$H_{\mathrm{C}} = \phi_r H_{\mathrm{C}}\phi_r + \psi_r H_{\mathrm{C}}\psi_r - L_{\phi_r} - L_{\psi_r}\,,$$

where L_{ϕ_r} and L_{ψ_r} are given by (24) and (25) ($\mathcal{M} = \{1,2\}$). We multiply with ϕ_R and get that

$$\phi_R H_{\mathrm{C}}\phi_R = \phi_r H_{\mathrm{C}}\phi_r + \phi_R\psi_r H_{\mathrm{C}}\psi_r\phi_R - \phi_R(L_{\phi_r} + L_{\psi_r})\phi_R\,.$$

We have used that $\phi_R\phi_r = \phi_r$ since $R > 2r$. Now, let $\gamma_R = \chi(\phi_R H_{\mathrm{C}}\phi_R)$ be the projection onto the negative part of $\phi_R H_{\mathrm{C}}\phi_R$. Then, by the variational principle and Theorem 14 (with $m = 1$, $\ell = r$, $\Omega = B(0, 3r)$, and $\theta = \phi_r$ and ψ_r, respectively),

$$\begin{aligned} &\mathrm{Tr}[\phi_R H_{\mathrm{C}}\phi_R]_- \\ &\quad = \mathrm{Tr}[\gamma_R\phi_r H_{\mathrm{C}}\phi_r] + \mathrm{Tr}[\gamma_R\phi_R\psi_r H_{\mathrm{C}}\psi_r\phi_R] - \mathrm{Tr}[\gamma_R\phi_R(L_{\phi_r} + L_{\psi_r})\phi_R] \\ &\quad \ge \mathrm{Tr}[\gamma_R\phi_r(H_{\mathrm{C}} - Cr^{-2})\phi_r] + \mathrm{Tr}[\gamma_R\phi_R\psi_r(H_{\mathrm{C}} - Cr^{-2}\phi_{3r})\psi_r\phi_R] \\ &\qquad - Cr^{-2}\,. \end{aligned} \tag{65}$$

Here, C is independent of α. We treat the part of the localisation error coming from the first term in (65). We split $H_{\mathrm{C}} = (1-\varepsilon)H_{\mathrm{C}} + \varepsilon H_{\mathrm{C}}$ for some $0<\varepsilon<1$ to be chosen and use the second term to control the error term.

By Theorem 16 (with $M=1$, $R_0=0$, $d(x)=|x|$, $m=1$ and $\nu=1$),

$$\begin{aligned}
&\mathrm{Tr}[\gamma_R\phi_r(\varepsilon H_{\mathrm{C}} - Cr^{-2})\phi_r]\\
&\quad= \varepsilon\,\mathrm{Tr}\big[(\phi_r\gamma_R\phi_r)\big\{\sqrt{-\alpha^{-2}\Delta+\alpha^{-4}} - \alpha^{-2} - (|\hat{x}|^{-1} + Cr^{-2}\varepsilon^{-1})\big\}\big]\\
&\quad\geq -C\varepsilon\Big(\alpha^{1/2} + \int\limits_{\alpha<|x|<2r}(|x|^{-1}+C\varepsilon^{-1}r^{-2})^{5/2}\,dx + \alpha^3\int\limits_{\alpha<|x|<2r}(|x|^{-1}+C\varepsilon^{-1}r^{-2})^4\,dx\Big)\\
&\quad\geq -C\varepsilon\Big(1 + r^{1/2} + \varepsilon^{-5/2}r^{-2} + \varepsilon^{-4}r^{-5}\big),
\end{aligned}$$

assuming $\varepsilon^{-1}r^{-2} \leq C\alpha^{-1}$ and using that $\alpha \leq 2/\pi$. We may choose $\varepsilon = r^{-1}$ if we assume that $r>1$ (note that then indeed $\varepsilon^{-1}r^{-2} = r^{-1} < 1 \leq 2\alpha^{-1}/\pi$). We then obtain

$$\mathrm{Tr}[\gamma_R\phi_r(\varepsilon H_{\mathrm{C}} - Cr^{-2})\phi_r] \geq -Cr^{-1/2}.$$

As a result, we have shown that

$$\begin{aligned}
&\mathrm{Tr}[\phi_R H_{\mathrm{C}}\phi_R]_-\\
&\quad\geq (1-\varepsilon)\,\mathrm{Tr}[\gamma_R\,\phi_r H_{\mathrm{C}}\phi_r] + \mathrm{Tr}[\gamma_R\phi_R\psi_r(H_{\mathrm{C}} - Cr^{-2}\phi_{3r})\psi_r\phi_R] - Cr^{-1/2}\\
&\quad\geq \mathrm{Tr}[\phi_r H_{\mathrm{C}}\phi_r]_- + \mathrm{Tr}[\phi_R\psi_r(H_{\mathrm{C}} - Cr^{-2}\phi_{3r})\psi_r\phi_R]_- - Cr^{-1/2}\,.
\end{aligned}$$

We will treat the term $\mathrm{Tr}[\phi_R\psi_r(H_{\mathrm{C}} - Cr^{-2}\phi_{3r})\psi_r\phi_R]_-$ by our semi-classical estimates in Section 5 below. We first rescale. Define the unitary scaling operator $(U\varphi)(x) = R^{-3/2}\varphi(R^{-1}x)$. Then

$$\begin{aligned}
\widetilde{H}_{\mathrm{C}} &:= U^*(H_{\mathrm{C}} - Cr^{-2}\phi_{3r})U\\
&= R^{-1}\big(\sqrt{-\alpha^{-2}\Delta + R^2\alpha^{-4}} - R\alpha^{-2} - |\hat{x}|^{-1} - CRr^{-2}\phi_{3r/R}(\hat{x})\big)\\
&= R^{-1}\big(T_\beta(-\mathrm{i}h\nabla) - |\hat{x}|^{-1} - CRr^{-2}\phi_{3r/R}(\hat{x})\big) \qquad (66)
\end{aligned}$$

with $\beta = \alpha^2R^{-1}\,(<R^{-1})$ and $h = R^{-1/2}$. Let $\phi_{R,r} = \phi_R\psi_r = \phi_R\sqrt{1-\phi_r^2}$ and $\psi(x) = \phi_{R,r}(Rx)$ (see (3) for T_β). In this way, $\phi_R\psi_r(H_{\mathrm{C}} - Cr^{-2}\phi_{3r})\psi_r\phi_R$ and $\psi\widetilde{H}_{\mathrm{C}}\psi$ are unitarily equivalent.

Now, let ℓ and φ_u be the functions in (56) and (60), respectively, when $M=1$, $r_1=0$, and $\ell_0 = h^2 = R^{-1}$. By another relativistic IMS localisation we get that

$$\begin{aligned}
\psi\widetilde{H}_{\mathrm{C}}\psi &= R^{-1}\int\limits_{r/3R<|u|<5/2}\psi\varphi_u\big(T_\beta(-\mathrm{i}h\nabla) - |\hat{x}|^{-1} - CRr^{-2}\phi_{3r/R}(\hat{x})\big)\varphi_u\psi\,\ell(u)^{-3}\,du\\
&\quad - R^{-1}\int\limits_{r/3R<|u|<5/2}\psi L_{\varphi_u}\psi\,\ell(u)^{-3}\,du\,.
\end{aligned}$$

We have used that $\psi\varphi_u = 0$ for $|u|\notin[r/3R, 5/2]$, since $\ell(u) \leq \frac{1}{2}(|u|^2+\ell_0^2)^{1/2}$ (see (58)) and $\operatorname{supp}\psi \subset \{r/R \leq |x| \leq 2\}$, $\operatorname{supp}\varphi_u \subset \{|x-u|\leq \ell(u)\}$.

Concerning L_{φ_u}, Theorem 14 with $\ell = \ell(u)/2$, $m=R$, and $\Omega = \Omega_u = \{|x-u| \leq 3\ell(u)/2\}$ gives

$$L_{\varphi_u} \leq CR^{-1}\ell(u)^{-2}\chi_{\Omega_u} + Q_{\varphi_u}\,,$$

with

$$\mathrm{Tr}[Q_{\varphi_u}] \le CR\alpha^{-1}\ell(u)^{-1}\mathrm{e}^{-\alpha^{-1}R\ell(u)/2}\,. \tag{67}$$

Here we have used (60).

Notice that if the supports of φ_u and $\varphi_{u'}$ overlap then $|u-u'| \le \ell(u)+\ell(u')$ and thus

$$\ell(u') \le \ell(u) + \|\nabla\ell\|_\infty(\ell(u)+\ell(u'))\,. \tag{68}$$

Therefore, since $\|\nabla\ell\|_\infty < 1/2$, we have that $\ell(u') \le C\ell(u)$ and thus $\ell(u)^{-1} \le C\ell(u')^{-1}$. Similarly, $\ell(u) \le C\ell(u')$, and so $\chi_{\Omega_u} \le \chi_{\{|x-u|\le C\ell(u')\}}$ if the supports of φ_u and $\varphi_{u'}$ overlap.

Using this and (60) we get for all $x \in \mathbb{R}^3$

$$\begin{aligned}\int \big(\ell(u)^{-2}\chi_{\Omega_u}(x)\big)\,\ell(u)^{-3}\,du \;&=\; \int \big(\ell(u)^{-2}\chi_{\Omega_u}(x)\big)\,\Big(\int \varphi_{u'}^2(x)\,\ell(u')^{-3}\,du'\Big)\,\ell(u)^{-3}\,du\\ &\le\; C\int \varphi_{u'}(x)\ell(u')^{-2}\varphi_{u'}(x)\,\ell(u')^{-3}\,du'.\end{aligned} \tag{69}$$

Rewriting the last integral with u as integration variable we get

$$\begin{aligned}\psi\widetilde{H}_{\mathrm{C}}\psi \;\ge\; & R^{-1}\int \psi\varphi_u\big(T_\beta(-\mathrm{i}h\nabla) - |\hat{x}|^{-1} - Ch^2\ell(u)^{-2}\big)\varphi_u\psi\,\ell(u)^{-3}\,du\\ & - R^{-1}\int \psi Q_{\varphi_u}\psi\,\ell(u)^{-3}\,du.\end{aligned}$$

Here we have also used that $Rr^{-2}\phi_{3r/R}(x) \le Ch^2\ell(u)^{-2}$ for x in the support of φ_u. This is a consequence of $\ell(u) \le \frac{1}{2}|u| + \frac{1}{2}\ell_0 \le \frac{1}{2}|x| + \frac{1}{2}\ell(u) + \ell_0$ for x in the support of φ_u which implies that $\ell(u) \le |x| + \ell_0 \le Cr/R$ for x in the support of φ_u and $\phi_{3r/R}$.

We will now use Theorem 23 (with $\phi = \psi\varphi_u$, $\ell = \ell(u)$, $B_\ell = \{|x-u| \le \ell(u)\}$, $f = f(u) = |u|^{-1/2}$) on

$$\psi\varphi_u\big(T_\beta(-\mathrm{i}h\nabla) - |\hat{x}|^{-1} - Ch^2\ell(u)^{-2}\big)\varphi_u\psi\,,$$

for u fixed with $|u| \in [r/3R, 5/2]$. We claim that

$$\|\partial_x^\eta(\psi\varphi_u)\|_\infty \le C_\eta\ell(u)^{-|\eta|} \text{ for all } \eta \in \mathbb{N}^3\,. \tag{70}$$

This follows from (60), (61), and the estimate $|\partial^\eta\psi(x)| \le C_\eta|x|^{-|\eta|}$. It suffices to check the latter for $1 \le |x| \le 2$ and $r/R \le |x| \le 2r/R$, due to the support properties of ψ. Furthermore, for $r > 3$, $|x|^{-1} + Ch^2\ell(u)^{-2}$ is smooth (as a function of x) on B_ℓ (use (58), $\ell_0 = R^{-1}$, and $|u| \ge r/3R$), and satisfies

$$\sup_{|x-u|<\ell(u)} \big|\partial_x^\eta(|x|^{-1} + Ch^2\ell(u)^{-2})\big| \le C_\eta f(u)^2\ell(u)^{-|\eta|} \text{ for all } \eta \in \mathbb{N}^3\,, \tag{71}$$

with $f(u) = |u|^{-1/2}$. For the Coulomb potential, this is trivial. For the other term, only the statement for $\eta = 0$ is non-trivial; it follows from (59), $h = R^{-1/2}$, and $|u| \ge r/3R$. Finally, the condition $f(u)^2\beta \le 1$ is also satisfied (when $r \ge 3$), since $|u| \ge r/3R$ and $\beta < R^{-1}$.

From Theorem 23 we conclude that

$$
\begin{aligned}
&\mathrm{Tr}[\phi_R\psi_r(H_{\mathrm{C}}-Cr^{-2}\phi_{3r})\psi_r\phi_R]_- = \mathrm{Tr}[\psi\widetilde{H}_{\mathrm{C}}\psi]_-\\
&\quad\geq R^{-1}(2\pi h)^{-3}\int\limits_{r/3R<|u|<5/2}\psi(v)^2\varphi_u(v)^2\left[T_\beta(q)-|v|^{-1}-Ch^2\ell(u)^{-2}\right]_-\ell(u)^{-3}\,dudvdq\\
&\qquad - CR^{-1}h^{-2+1/5}\int\limits_{r/3R<|u|<5/2} f(u)^{4-1/5}\ell(u)^{-1-1/5}\,du\\
&\qquad - R^{-1}\int\limits_{r/3R<|u|<5/2}\mathrm{Tr}\big[\psi Q_{\varphi_u}\psi\big]\,\ell(u)^{-3}\,du\,.
\end{aligned}
$$

Integrating the semi-classical error using $f(u)=|u|^{-1/2}$, (59), and $R>r$ gives the lower bound $-CR^{-1}h^{-2+1/5}(R/r)^{1/10} = -\,Cr^{-1/10}$.

From (67) it follows, using (59), $\alpha\leq 2/\pi$, and $R>r$, that

$$
\begin{aligned}
R^{-1}\int\limits_{r/3R<|u|<5/2}\mathrm{Tr}\big[\psi Q_{\varphi_u}\psi\big]\,\ell(u)^{-3}\,du \;&\leq\; C\int\limits_{r/3R<|u|<5/2}\alpha^{-2}\mathrm{e}^{-\alpha^{-1}R\ell(u)/2}\ell(u)^{-3}\,du\\
&\leq\; Cr^{-1}\mathrm{e}^{-r/8}\,.
\end{aligned}
$$

Since $\mathrm{supp}\,\varphi_u\subset\{v\,|\,|u-v|\leq\ell(u)\}$ and $|u|\leq 5/2$ we have $|v|\leq|u|+\ell(u)\leq C\ell(u)$ on $\mathrm{supp}\,\varphi_u$. Using this, integrating in u (using (60)), we get

$$
\begin{aligned}
&R^{-1}(2\pi h)^{-3}\int\limits_{r/3R<|u|<5/2}\psi(v)^2\varphi_u(v)^2\left[T_\beta(q)-|v|^{-1}-Ch^2\ell(u)^{-2}\right]_-\ell(u)^{-3}\,dudvdq\\
&\quad\geq\; R^{-1}\frac{1}{(2\pi h)^3}\int\psi(v)^2\left[\sqrt{\beta^{-1}q^2+\beta^{-2}}-\beta^{-1}-|v|^{-1}-Ch^2|v|^{-2}\right]_-\,dvdq\,.
\end{aligned}
$$

In order to compare this latter relativistic semi-classical expression with the non-relativistic semi-classical one we use the inequality $|x_- - y_-|\leq|x-y|$ and a Taylor expansion of $\sqrt{t^2+1}-1$ to arrive at

$$
\begin{aligned}
&\int\Big|\left[\tfrac12 q^2-a\right]_- - \left[\sqrt{\beta^{-1}q^2+\beta^{-2}}-\beta^{-1}-a-b\right]_-\Big|\,dq\\
&\qquad\leq\; C\beta(\beta(a+b)^2+2(a+b))^{7/2}+Cb(\beta(a+b)^2+2(a+b))^{3/2} \qquad (72)
\end{aligned}
$$

for all $a,b>0$. This gives, using $h^2=R^{-1}$ and $\beta<R^{-1}$, that

$$
\begin{aligned}
&\left|\int\psi(v)^2\left(\left[\tfrac12 q^2-|v|^{-1}\right]_- - \left[\sqrt{\beta^{-1}q^2+\beta^{-2}}-\beta^{-1}-|v|^{-1}-Ch^2|v|^{-2}\right]_-\right)dvdq\right|\\
&\qquad\leq\; CR^{-1}\int\limits_{r/R<|v|<2}|v|^{-7/2}\,dv\;\leq\; C(Rr)^{-1/2}\,, \qquad (73)
\end{aligned}
$$

since $R>r\geq 1$.

Thus undoing the scaling we arrive at

$$
\begin{aligned}
&R^{-1}(2\pi h)^{-3}\int\limits_{r/3R<|u|<5/2}\psi(v)^2\varphi_u(v)^2\left[T_\beta(q)-|v|^{-1}-Ch^2\ell(u)^{-2}\right]_-\ell(u)^{-3}\,dudvdq\\
&\qquad\geq\; (2\pi)^{-3}\int\phi_{R,r}(v)^2\left[\tfrac12 q^2-|v|^{-1}\right]_-\,dvdq - Cr^{-1/10}\,.
\end{aligned}
$$

Summarizing, we have proved that there exists a constant $C = C(\phi)$, independent of $\alpha \in [0, 2/\pi]$, such that for r large enough, and $R > 2r$,

$$\begin{aligned}&\mathrm{Tr}[\phi_R H_{\mathrm{C}} \phi_R]_- \\ &\quad\geq \mathrm{Tr}[\phi_r H_{\mathrm{C}} \phi_r]_- + (2\pi)^{-3} \int \phi_{R,r}(v)^2 \left[\tfrac{1}{2}q^2 - |v|^{-1}\right]_- dvdq - Cr^{-1/10}\,. \end{aligned} \tag{74}$$

Next, we want to bound $\mathrm{Tr}[\phi_R H_{\mathrm{C}} \phi_R]_-$ from above by $\mathrm{Tr}[\phi_r H_{\mathrm{C}} \phi_r]_-$ by constructing a density matrix. To this end, we first set $\gamma_r = \chi(\phi_r H_{\mathrm{C}} \phi_r)$. Then we let $\widetilde{\gamma}_u$ be the density matrix we get when we use Theorem 23 for the rescaled operator $\psi\varphi_u \widetilde{H}_{\mathrm{C}} \varphi_u \psi$ (now with $\widetilde{H}_{\mathrm{C}} = U^* H_{\mathrm{C}} U$ with U as in (66)), for fixed u with $|u| \in [r/3R, 5/2]$, and set $\gamma_u = U\varphi_u \widetilde{\gamma}_u \varphi_u U^*$. Finally, we define

$$\gamma = \phi_r \gamma_r \phi_r + \int_{r/3R<|u|<5/2} \psi_r\, \gamma_u\, \psi_r\, \ell(u)^{-3}\, du\,. \tag{75}$$

Since $\mathbf{0} \leq \widetilde{\gamma} \leq \mathbf{1}$ and $\int \varphi_u^2(x)\ell(u)^{-3}\,du = 1$,

$$\mathbf{0} \leq \int \gamma_u\, \ell(u)^{-3}\, du \leq \mathbf{1}\,,$$

and so we see, by multiplication with ψ_r on both sides, that $\mathbf{0} \leq \gamma \leq \mathbf{1}$. Also, γ is trivially trace class. By the variational principle we obtain that

$$\begin{aligned}\mathrm{Tr}[\phi_R H_{\mathrm{C}} \phi_R]_- &\leq \mathrm{Tr}[\phi_R H_{\mathrm{C}} \phi_R \gamma] \\ &= \mathrm{Tr}\big[\phi_R \phi_r H_{\mathrm{C}} \phi_r \phi_R\, \chi(\phi_r H_{\mathrm{C}} \phi_r)\big] \\ &\quad + \int_{r/3R<|u|<5/2} \mathrm{Tr}[\psi_r \phi_R H_{\mathrm{C}} \phi_R \psi_r \gamma_u]\, \ell(u)^{-3}\, du \\ &\leq \mathrm{Tr}[\phi_r H_{\mathrm{C}} \phi_r]_- + \int_{r/3R<|u|<5/2} \mathrm{Tr}[\psi\varphi_u \widetilde{H}_{\mathrm{C}} \varphi_u \psi \widetilde{\gamma}_u]\, \ell(u)^{-3}\, du\,.\end{aligned}$$

Here we have used that $\phi_R\phi_r H_{\mathrm{C}} \phi_r \phi_R = \phi_r H_{\mathrm{C}} \phi_r$, since $R > 2r$, and again scaled the operators inside the trace in the integrand. Using Theorem 23 we can bound the integral from above by

$$\begin{aligned}R^{-1}(2\pi h)^{-3} \int \psi(v)^2 \varphi_u(v)^2 \big[T_\beta(q) - |v|^{-1}\big]_- \ell(u)^{-3}\, dudvdq \\ + CR^{-1}h^{-2+1/5} \int_{r/3R<|u|<5/2} f(u)^{4-1/5} \ell(u)^{-1-1/5}\, du\,.\end{aligned}$$

As in the case of the lower bound, the error term is bounded by $Cr^{-1/10}$.

Integrating with respect to u in the semi-classical expression above, changing back coordinates, and using (73), we conclude that

$$\mathrm{Tr}[\phi_R H_{\mathrm{C}} \phi_R]_- \leq \mathrm{Tr}[\phi_r H_{\mathrm{C}} \phi_r]_- + (2\pi)^{-3} \int \phi_{R,r}(v)^2 \big[\tfrac{1}{2}q^2 - |v|^{-1}\big]_-\, dvdq + Cr^{-1/10}\,. \tag{76}$$

Combining (74) and (76) we have shown that for $R > 2r$,

$$
\begin{aligned}
&\big|S_R - S_r\big| \\
&\leq \Big|\mathrm{Tr}[\phi_R H_{\mathrm{C}} \phi_R]_- - \mathrm{Tr}[\phi_r H_{\mathrm{C}} \phi_r]_- + (2\pi)^{-3} \int \big(\phi_r(v)^2 - \phi_R(v)^2\big) \left[\tfrac{1}{2}q^2 - |v|^{-1}\right]_- dv dq\Big| \\
&\leq Cr^{-1/10} .
\end{aligned}
$$

Hence, $\{S_n\}_{n\in\mathbb{N}}$ is a Cauchy-sequence and with $\mathcal{S} = \mathcal{S}(\alpha)$ the limiting value we have

$$
\big|S_r - \mathcal{S}\big| \leq Cr^{-1/10} .
$$

This proves (62). That $\mathcal{S}$ is non-increasing follows from the fact that $T_{\alpha^2}(p)$ (see (3)) is decreasing in α. Finally, that $\mathcal{S}(0) = 1/4$ is a well-known fact [36]. □

Proof of Theorem 4. Using the combined Daubechies-Lieb-Yau inequality (see Theorem 16) with $\alpha = \beta^{1/2}h^{-1}(\leq 1)$ and $m = h^{-2}$ we may assume that h is bounded by some constant, which we may choose small depending on M and r_0, using that $z_k \leq 2/\pi$, $k = 1, \ldots, M$, and that $\mathcal{S}$ is a bounded function (since it is non-increasing; see Lemma 25).

In order to control the region close to and far away from all the nuclei we introduce localisation functions $\theta_\pm \in C^1(\mathbb{R})$ with the properties that $0 \leq \theta_\pm \leq 1$ and

(1) $\theta_-^2 + \theta_+^2 = 1$,
(2) $\theta_-(t) = 1$ if $t < 1$ and $\theta_-(t) = 0$ for $t > 2$.

Let $0 < r < r_0/4$ and $0 < r_0 < R$ and define $\Phi_\pm(x) = \theta_\pm(d(x)/R)$ and $\phi_\pm(x) = \theta_\pm(d(x)/r)$ (with $d = d_{\mathbf{r}}$ as in (4)). We choose (assuming h is small enough)

$$
r = \delta^{-1}h^2 \quad \text{and} \quad R = \begin{cases} Ch^{-1}, & \text{if } \mu = 0 \\ R_\mu, & \text{if } \mu \neq 0 \end{cases} , \tag{77}
$$

where $\delta = h < 1/2$ and $R_\mu = C\mu^{-1}$ is chosen such that $-V(x) \geq 0$ for $d(x) \geq R_\mu$ (see (5)). We will keep writing δ and R in the calculations below to show why these choices are optimal. Clearly, $\Phi_-^2 + \Phi_+^2 = 1$, $\phi_-^2 + \phi_+^2 = 1$, and $\phi_-^2 + \Phi_-^2\phi_+^2 + \Phi_+^2 = 1$. Note also that

$$
\phi_-(x) = \sum_{k=1}^{M} \theta_{r,k}(x) \quad \text{with} \quad \theta_{r,k}(x) = \theta_-(|x - r_k|/r) .
$$

Step 1: Lower bound on the quantum energy.

By the relativistic IMS formula (23) and Theorem 14 with $m = h^{-2}$, $\alpha = \beta^{1/2}h^{-1}(\leq 1)$, and either $\ell = R$, $\Omega = \{d(x) \leq 3R\}$, and $\theta = \Phi_\pm$ respectively, or $\ell = r$, $\Omega = \{d(x) \leq 3r\}$, and $\theta = \theta_{r,k}$, $k = 1, \ldots, M$, or $\theta = \phi_+$ respectively, we find that

$$
\begin{aligned}
&T_\beta(-\mathrm{i}h\nabla) - V(\hat{x}) \\
&= \Phi_+\big(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x})\big)\Phi_+ + \Phi_-\big(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x})\big)\Phi_- - L_{\Phi_-} - L_{\Phi_+} \\
&= \sum_{k=1}^{M} \theta_{r,k}\big(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x})\big)\theta_{r,k} + \Phi_-\phi_+\big(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x})\big)\phi_+\Phi_- \\
&\quad + \Phi_+\big(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x})\big)\Phi_+ - \Phi_-\big(\sum_{k=1}^{M} L_{\theta_{r,k}} + L_{\phi_+}\big)\Phi_- - L_{\Phi_-} - L_{\Phi_+} ,
\end{aligned} \tag{78}
$$

with

$$
\begin{aligned}
L_{\Phi_\pm} &\leq Ch^2\|\nabla\Phi_\pm\|_\infty^2 \chi_{\{d(x)\leq 3R\}} + Q_{\Phi_\pm} , &(79)\\
\mathrm{Tr}[Q_{\Phi_\pm}] &\leq C\beta^{-1}R^{-1}\mathrm{e}^{-(\beta^{1/2}h)^{-1}R} \|\nabla\Phi_\pm\|_\infty^2 \big|\{d(x) \leq 3R\}\big| , &(80)
\end{aligned}
$$

and (with, by abuse of notation, $L_{\phi_-} = \sum_{k=1}^{M} L_{\theta_{r,k}}$)

$$\begin{aligned} L_{\phi_\pm} &\leq Ch^2\|\nabla\phi_\pm\|_\infty^2\,\chi_{\{d(x)\leq 3r\}} + Q_{\phi_\pm}\,, & (81)\\ \mathrm{Tr}[Q_{\phi_\pm}] &\leq C\beta^{-1}r^{-1}\mathrm{e}^{-(\beta^{1/2}h)^{-1}r}\,\|\nabla\phi_\pm\|_\infty^2\,\big|\{d(x)\leq 3r\}\big|\,. & (82)\end{aligned}$$

Using $\big|\{d(x)\leq 3R\}\big| \leq 36\pi MR^3$, $\|\nabla\Phi_\pm\|_\infty \leq CR^{-1}$ (and the corresponding estimates for r and $\phi_\pm$), $\beta \leq h^2$, and h small, it follows that

$$\mathrm{Tr}[Q_{\Phi_\pm}] \leq Ch^2R^{-2}\mathrm{e}^{-h^{-2}R/2} \leq C_Nh^N, \quad \mathrm{Tr}[Q_{\phi_\pm}] \leq Ch^2r^{-2}\mathrm{e}^{-h^{-2}r/2} \leq C_Nh^N\,,$$

for any $N > 0$ by the choices (77).

Hence we have that

$$\begin{aligned} &\mathrm{Tr}\big[T_\beta(-\mathrm{i}h\nabla) - V(\hat{x})\big]_-\\ &\geq \sum_{k=1}^{M}\mathrm{Tr}\big[\theta_{r,k}\big(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x}) - Ch^2r^{-2}\big)\theta_{r,k}\big]_-\\ &\quad + \mathrm{Tr}\big[\Phi_-\phi_+\big(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x}) - Ch^2r^{-2}\chi_{\{d(x)\leq 3r\}} - Ch^2R^{-2}\big)\phi_+\Phi_-\big]_-\\ &\quad + \mathrm{Tr}\big[\Phi_+\big(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x}) - Ch^2R^{-2}\chi_{\{d(x)\leq 3R\}}\big)\Phi_+\big]_- - Ch^{-2+1/10}\,. \qquad (83)\end{aligned}$$

Each of the first three terms above will be compared to the corresponding semi-classical expression. We shall treat the three terms by different methods. The first term will be calculated using the Scott correction for Hydrogen in Lemma 25. The second term will be computed using the local rescaled semi-classics in Theorem 23. The last term is an error term which we will treat first.

Control of the third term in (83)**.**

We use the Daubechies inequality (17) with $m = h^{-2}$ and $\alpha = \beta^{1/2}h^{-1}(\leq 1)$. In the case $\mu = 0$ we obtain, using the choice (77) of R,

$$\begin{aligned} &\mathrm{Tr}\big[\Phi_+(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x}) - Ch^2R^{-2}\chi_{\{d(x)\leq 3R\}})\Phi_+\big]_-\\ &\geq\; -Ch^{-3}M\int_{|x|>R}|x|^{-15/2}\,dx - CM\int_{|x|>R}|x|^{-12}\,dx - Ch^2R^{-2} - Ch^8R^{-5}\\ &\geq\; -C\big(h^{-3}R^{-9/2} + R^{-9} + h^2R^{-2} - h^8R^{-5}\big) \geq -Ch^{3/2}\,. \qquad (84)\end{aligned}$$

The case $\mu \neq 0$ gives a smaller error since $-V \geq 0$ on the support of Φ_+ in this case.

Control of the first term in (83)**.**

Using (6) and (77) we have

$$\begin{aligned} &\sum_{k=1}^{M}\mathrm{Tr}\big[\theta_{r,k}\big(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x}) - Ch^2r^{-2}\big)\theta_{r,k}\big]_-\\ &\qquad \geq \sum_{k=1}^{M}\mathrm{Tr}\,\big[\theta_r\big(T_\beta(-\mathrm{i}h\nabla) - z_k|\hat{x}|^{-1} - C\delta^2h^{-2}\big)\theta_r\big]_-\,,\end{aligned}$$

where we have written $\theta_r(x) = \theta_-(|x|/r)$. We have used here that

$$Cr_{\min}^{-1} + C \leq Cr_0^{-1} + C \leq C\delta^2h^{-2}\,. \qquad (85)$$

It is this relation which sets a lower bound on δ. We will control the error using the combined Daubechies-Lieb-Yau inequality in Theorem 16 with $m = h^{-2}$ and $\alpha = \beta^{1/2}h^{-1}(\leq 1)$. Note that $m\alpha^{-1} = \beta^{-1/2}h^{-1} \geq h^{-2}$. Thus using Theorem 16 we find, for all density matrices γ and all $\varepsilon \geq \delta^2$, that

$$\varepsilon \operatorname{Tr}\left[\gamma\big(\theta_r(T_\beta(-\mathrm{i}h\nabla) - z_k|\hat{x}|^{-1} - C\varepsilon^{-1}\delta^2 h^{-2})\theta_r\big)\right] \geq -C(\varepsilon\delta^{-1/2} + \varepsilon^{-3/2}\delta^2 + \varepsilon^{-3}\delta^5)h^{-2}.$$

Thus for all density matrices γ and all $\varepsilon \geq \delta^2$ we have

$$C\delta^2 h^{-2}\operatorname{Tr}[\gamma\theta_r^2] \leq \varepsilon \operatorname{Tr}\left[\gamma\theta_r(T_\beta(-\mathrm{i}h\nabla) - z_k|\hat{x}|^{-1})\theta_r\right] + C(\varepsilon\delta^{-1/2} + \varepsilon^{-3/2}\delta^2 + \varepsilon^{-3}\delta^5)h^{-2}\,. \quad (86)$$

Hence

$$\begin{aligned}&\sum_{k=1}^{M}\operatorname{Tr}\big[\theta_{r,k}\big(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x}) - Ch^2r^{-2}\big)\theta_{r,k}\big]_- \qquad (87)\\ &\quad\geq (1-\varepsilon)\sum_{k=1}^{M}\operatorname{Tr}\big[\theta_r(T_\beta(-\mathrm{i}h\nabla) - z_k|\hat{x}|^{-1})\theta_r\big]_- - C(\varepsilon\delta^{-1/2} + \varepsilon^{-3/2}\delta^2 + \varepsilon^{-3}\delta^5)h^{-2}\,.\end{aligned}$$

For the corresponding semi-classical expression we have from (6) and (85) (using $\delta < 1/2$ and $|x_- - y_-| \leq |x-y|$) that

$$\begin{aligned}&\left|(2\pi h)^{-3}\int \phi_-(v)^2\big[\tfrac{1}{2}p^2 - V(v)\big]_-\,dvdp - \sum_{k=1}^{M}(2\pi h)^{-3}\int \theta_r(v)^2\big[\tfrac12 p^2 - z_k|v|^{-1}\big]_-\,dvdp\right|\\ &\qquad\leq C\delta^{1/2}h^{-2}. \qquad (88)\end{aligned}$$

A simple rescaling applied to the local Hydrogen result in Lemma 25 gives that

$$\begin{aligned}&\Big|\operatorname{Tr}\big[\theta_r(T_\beta(-\mathrm{i}h\nabla) - z_k|\hat{x}|^{-1})\theta_r\big]_- - (2\pi h)^{-3}\int \theta_r(v)^2\big[\tfrac12 p^2 - z_k|v|^{-1}\big]_-\,dvdp\\ &\qquad - z_k^2h^{-2}\mathcal{S}(\beta^{1/2}h^{-1}z_k)\Big| \leq Ch^{-2}(h^{-2}r)^{-1/10} = Ch^{-2}\delta^{1/10}. \qquad (89)\end{aligned}$$

Combining (87), (88), and (89), using that $\mathcal{S}$ is a bounded function (since it is non-increasing; see Lemma 25), that $\delta < 1/2$, and that

$$(2\pi h)^{-3}\int \theta_r(v)^2\big[\tfrac12 p^2 - z_k|v|^{-1}\big]_-\,dvdp \leq Ch^{-3}r^{1/2} = Ch^{-2}\delta^{-1/2}\,,$$

and choosing $\varepsilon = \delta$, we conclude that

$$\begin{aligned}\operatorname{Tr}\big[\phi_-\big(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x}) - Ch^2r^{-2}\big)\phi_-\big]_- \;\geq\;& (2\pi h)^{-3}\int \phi_-(v)^2\big[\tfrac12 q^2 - V(v)\big]_-\,dvdq\\ &+ h^{-2}\sum_{k=1}^{M} z_k^2\mathcal{S}(\beta^{1/2}h^{-1}z_k) - C\delta^{1/10}h^{-2}. \qquad (90)\end{aligned}$$

Control of the second term in (83)**.**

Here we use the local rescaled semi-classics in Theorem 23. Before we apply our semi-classical estimates on the support of $\Phi_-\phi_+$ we localise using the functions φ_u from (60) for general M and with $\ell(u)$ as in (56), with $\ell_0 = r/4$. From (77) and the choice of δ it follows that $\ell_0 < 1$ for h small enough. If x is in the support of $\Phi_-\phi_+$ and in the support of φ_u then $d(u) > r/2 = 2\ell_0$ since (using (58))

$$r \leq d(x) \leq d(u) + \ell(u) < d(u) + \max\{d(u), \ell_0\}\,,$$

and also $d(u) \le 2R+1$ since $\ell(u) < 1/2$. Using again the relativistic IMS localisation (23) we thus have

$$
\begin{aligned}
&\Phi_-\phi_+\big(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x}) - Ch^2r^{-2}\chi_{\{d(x)\le 3r\}} - Ch^2R^{-2}\big)\phi_+\Phi_- \\
&\quad = \int\limits_{r/2<d(u)<2R+1} \Phi_-\phi_+\varphi_u\big(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x}) - Ch^2r^{-2}\chi_{\{d(x)\le 3r\}} - Ch^2R^{-2}\big)\varphi_u\phi_+\Phi_-\,\ell(u)^{-3}\,du \\
&\qquad - \int\limits_{r/2<d(u)<2R+1} \Phi_-\phi_+L_{\varphi_u}\phi_+\Phi_-\ell(u)^{-3}\,du\,. \qquad (91)
\end{aligned}
$$

Concerning L_{φ_u}, Theorem 14 with $\ell = \ell(u)/2$ and $\Omega = \Omega_u = \{|x-u| \le 3\ell(u)/2\}$ (and $m = h^{-2}$ and $\alpha = \beta^{1/2}h^{-1}(\le 1)$) gives, using (29), that

$$
L_{\varphi_u} \le Ch^2\ell(u)^{-2}\chi_{\Omega_u} + Q_{\varphi_u}\,, \qquad (92)
$$

with

$$
\mathrm{Tr}[Q_{\varphi_u}] \le C\beta^{-1}\mathrm{e}^{-(\beta^{1/2}h)^{-1}\ell(u)} \le C_Nh^N \qquad (93)
$$

for all $N > 0$ as a consequence of $\ell(u) \ge (1+M)^{-1}r/8$ and $\beta \le h^2$. Thus

$$
\mathrm{Tr}\Big[\int\limits_{r/2<d(u)<2R+1} \Phi_-\phi_+Q_{\varphi_u}\phi_+\Phi_-\ell(u)^{-3}\,du\Big] \;\le\; C_Nh^N \;\text{ for all } N>0\,.
$$

By the same arguments as in the proof of Lemma 25 above (see (68) and (69)) we join the new localisation error term (from (91), (92)) with the previous localisation errors from (79) and (81). Since $\ell(u) \le \max\{d(u), r/4\}$ we have $R^{-2} \le C\ell(u)^{-2}$ for $d(u) \le 2R+1$ (and h small enough when $\mu = 0$; for $\mu \ne 0$, use $\ell(u) < 1/2$) and, by (61) (valid on the support of φ_u when $d(u) > r/2 = 2\ell_0$),

$$
r^{-2}\chi_{\{d(x)\le 3r\}}(x)\varphi_u(x)^2 \le C\ell(u)^{-2}\varphi_u(x)^2\,.
$$

This way, we have proved that

$$
\begin{aligned}
&\mathrm{Tr}\big[\Phi_-\phi_+\big(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x}) - Ch^2r^{-2}\chi_{\{d(x)\le 3r\}} - Ch^2R^{-2}\big)\phi_+\Phi_-\big]_- \qquad (94)\\
&\ge \int\limits_{r/2<d(u)<2R+1} \mathrm{Tr}\big[\phi_+\varphi_u\left(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x}) - Ch^2\ell(u)^{-2}\right)\varphi_u\phi_+\big]_-\,\ell(u)^{-3}\,du \;-\; Ch^{-2+1/10}\,.
\end{aligned}
$$

Note that there is no need to write Φ_- on the right side, since in general $\mathrm{Tr}(\Phi A\Phi)_- \ge \mathrm{Tr}A_-$ for any self-adjoint operator A and any function $0 \le \Phi \le 1$.

For u such that $d(u) > r/2 = 2\ell_0$ and $d(u) < 2R+1$ we have from (5) and (77) that

$$
\sup_{|x-u|\le\ell(u)} |\partial^\eta(V(x) - Ch^2\ell(u)^{-2})| \le Cf(u)^2\ell(u)^{-|\eta|} \text{ for } |\eta| \le 3\,,
$$

$$
\|\partial^\eta(\phi_+\phi_u)\|_\infty \le C_\eta\ell(u)^{-|\eta|} \text{ for } |\eta| \le 7\,,
$$

with

$$
f(u) = \begin{cases} d(u)^{-1/2} & \text{if } \mu \ne 0 \\ \min\{d(u)^{-1/2}, d(u)^{-3/2}\} & \text{if } \mu = 0 \end{cases}. \qquad (95)
$$

We have also used that $d(u) \ge \delta^{-1}h^2/2 \ge h^2$ and $\min\{1, d(u)\} \le C\ell(u)$.

We are therefore in a position to use the rescaled semi-classics in Theorem 23 on the ball $\{|x-u| \le \ell\}$ with $\ell = \ell(u)$, $f = f(u)$, and $\phi = \phi_+\phi_u$ for each u with $r/2 \le d(u) \le 2R+1$.

Note in particular that $\beta f^2(u) \leq \beta d(u)^{-1} \leq 2\beta/r = 2\beta\delta h^{-2} \leq 2\delta \leq 1$. We conclude that for all u with $r/2 \leq d(u) \leq 2R+1$,

$$\begin{aligned} &\Big|\mathrm{Tr}\big[\phi_+\varphi_u\big(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x}) - Ch^2\ell(u)^{-2}\big)\varphi_u\phi_+\big]_- \\ &\qquad - (2\pi h)^{-3}\int \phi_+(v)^2\varphi_u(v)^2\big[\sqrt{\beta^{-1}q^2+\beta^{-2}} - \beta^{-1} - V(v) - Ch^2\ell(u)^{-2}\big]_-\,dvdq\Big| \\ &\leq \ Ch^{-2+1/5}f(u)^{4-1/5}\ell(u)^{2-1/5}. \end{aligned} \tag{96}$$

The semi-classical integral may be estimated using (72)

$$\begin{aligned} &\left|\int \big[\sqrt{\beta^{-1}q^2+\beta^{-2}} - \beta^{-1} - V(v) - Ch^2\ell(u)^{-2}\big]_-\,dq - \int \big[\tfrac12 q^2 - V(v)\big]_-\,dq\right| \\ &\quad\leq\ Ch^2\big(|V(v)| + h^2\ell(v)^{-2}\big)^{7/2} + Ch^2\ell(v)^{-2}\big(|V(v)| + h^2\ell(v)^{-2}\big)^{3/2} \\ &\quad\leq\ C\big(h^2|V(v)|^{7/2} + h^2\ell(v)^{-2}|V(v)|^{3/2} + (h\ell(v)^{-1})^5\big), \end{aligned} \tag{97}$$

for v in the support of φ_u, since then we have $\ell(v) \leq 3\ell(u)/2$ (see (57)) and $|V(v)| \leq Cd(v)^{-1} \leq Cd(u)^{-1} \leq Ch^{-2}$ (see (5), (61) and (58)). We have also used that $\beta \leq h^2$ and that, by (58) and (77) ($\ell_0 = r/4$), $h^2\ell(v)^{-2} \leq Ch^2r^{-2} = C\delta^2h^{-2} \leq Ch^{-2}$.

Combining (94), (96), and (97) (remembering that $d(u) \leq Cd(v)$ if v is in the support of φ_u and $d(u) > r/2 = 2\ell_0$) we find, using (60), (5), and (95), that

$$\begin{aligned} &\mathrm{Tr}\big[\Phi_-\phi_+\big(T_\beta(-\mathrm{i}h\nabla) - V(\hat{x}) - Ch^2r^{-2}\chi_{\{d(x)\leq 3r\}} - Ch^2R^{-2}\big)\phi_+\Phi_-\big]_- \\ &\quad\geq\ (2\pi h)^{-3}\int \phi_+(v)^2\big[\tfrac12 q^2 - V(v)\big]_-\,dq\,dv - C\int_{r/2<d(u)<2R+1} h^{-2+1/5}f(u)^{19/5}\ell(u)^{-6/5}\,du \\ &\qquad - C\int_{C^{-1}r<d(v)<2R+2} h^{-3}(h^2d(v)^{-7/2} + h^2\ell(v)^{-2}f(v)^3 + (h\ell(v)^{-1})^5)\,dv - Ch^{-2+1/10}. \end{aligned} \tag{98}$$

If $\mu \neq 0$ the error term in (98) is controlled as follows:

$$\begin{aligned} &\int_{C^{-1}r<d(v)<2R+2} \big(h^{-2+1/5}f(v)^{19/5}\ell(v)^{-6/5} + h^{-1}d(v)^{-7/2} + h^{-1}\ell(v)^{-2}f(v)^3 + h^2\ell(v)^{-5}\big)\,dv \\ &\quad\leq\ C\int_{C^{-1}r<|v|<2R+2} \big(h^{-2+1/5}|v|^{-19/10}\min\{1,|v|\}^{-6/5} + h^{-1}|v|^{-7/2} \\ &\qquad\qquad + h^{-1}\min\{1,|v|\}^{-2}|v|^{-3/2} + h^2\min\{1,|v|\}^{-5}\,\big)\,dv \\ &\quad\leq\ C\big(h^{-2+1/5}(R^{11/10} + r^{-1/10}) + h^{-1}r^{-1/2} + h^{-1}R^{3/2} + h^2R^3 + h^2r^{-2}\big) \\ &\quad\leq\ Ch^{-2+1/10}, \end{aligned} \tag{99}$$

with the choices (77) where $R = R_\mu$ is a constant.

If $\mu = 0$ we get instead

$$\begin{aligned} &\int_{C^{-1}r<d(v)<2R+2} \big(h^{-2+1/5}f(v)^{19/5}\ell(v)^{-6/5} + h^{-1}d(v)^{-7/2} + h^{-1}\ell(v)^{-2}f(v)^3 + h^2\ell(v)^{-5}\big)\,dv \\ &\qquad \leq C\big(h^{-2+1/5}r^{-1/10} + h^{-1}r^{-1/2} + h^2R^3 + h^2r^{-2}\big) \leq Ch^{-2+1/10}. \end{aligned} \tag{100}$$

If we insert the last two estimates (100) and (99) into (98) and then together with (84) and (90) into (83) we arrive at a lower bound on the quantum energy corresponding to one direction in (7).

Step 2: Upper bound on the quantum energy.

We obtain an upper bound on the quantum energy by choosing the density matrix

$$\gamma = \sum_{k=1}^{M} \theta_{r,k}\gamma_k\theta_{r,k} + \int\limits_{d(u)<2R+1} \phi_+\varphi_u\gamma_u\varphi_u\phi_+ \,\ell(u)^{-3}\,du\,, \tag{101}$$

where γ_k, $k=1,\dots,M$, are the density matrices

$$\gamma_k = \chi\big(\theta_{r,k}\big(T_\beta(-\mathrm{i}h\nabla) - z_k|\hat{x}-r_k|^{-1}\big)\theta_{r,k}\big)$$

and γ_u, $u\in\mathbb{R}^3$, are the density matrices given in Theorem 23 for the potential V with B_ℓ being the ball centered at u, $\ell=\ell(u)$, $f=f(u)$ (see (95)), and $\phi=\phi_+\varphi_u$. Since

$$\sum_{k=1}^{M}\theta_{r,k}^2 + \phi_+^2 = \phi_-^2+\phi_+^2 = 1\,, \tag{102}$$

we immediately see from (60) that γ is a density matrix.

Using this density matrix as a trial state we obtain from Theorem 23 that

$$\begin{aligned}
&\mathrm{Tr}\big[T_\beta(-\mathrm{i}h\nabla) - V(\hat{x})\big]_- \\
&\leq \sum_{k=1}^{M}\mathrm{Tr}\big[\theta_{r,k}\big(T_\beta(-\mathrm{i}h\nabla)-V(\hat{x})\big)\theta_{r,k}\big]_- \\
&\quad + (2\pi h)^{-3}\int\limits_{d(u)<2R+1} \phi_+(v)^2\varphi_u(v)^2\big[\sqrt{\beta^{-1}q^2+\beta^{-2}}-\beta^{-1}-V(v)\big]_-\ell(u)^{-3}\,dvdqdu \\
&\quad + Ch^{-2+1/5}\int\limits_{r/2<d(u)<2R+1} f(u)^{19/5}\ell(u)^{-6/5}\,du\,,
\end{aligned} \tag{103}$$

where we have used the fact that ϕ_+ and φ_u have overlapping supports only if $d(u)>r/2$. The last error term is estimated by $Ch^{-2+1/10}$ as in the lower bound.

Using that $\sqrt{\beta^{-1}q^2+\beta^{-2}}-\beta^{-1}\leq\frac{1}{2}q^2$ and the normalization of φ_u (60) we find that

$$\begin{aligned}
&(2\pi h)^{-3}\int\limits_{d(u)<2R+1} \phi_+(v)^2\varphi_u(v)^2\big[\sqrt{\beta^{-1}q^2+\beta^{-2}}-\beta^{-1}-V(v)\big]_-\ell(u)^{-3}\,dvdqdu \\
&\leq (2\pi h)^{-3}\int \phi_+(v)^2\big[\tfrac{1}{2}q^2-V(v)\big]_-\,dvdq \\
&\quad - (2\pi h)^{-3}\int\limits_{d(u)>2R+1}\phi_+(v)^2\varphi_u(v)^2\big[\tfrac{1}{2}q^2-V(v)\big]_-\ell(u)^{-3}\,dvdqdu \\
&\leq (2\pi h)^{-3}\int \phi_+(v)^2\big[\tfrac{1}{2}q^2-V(v)\big]_-\,dvdq + Ch^{-3}\int\limits_{d(v)>2R}|V(v)_-|^{5/2}\,dv\,.
\end{aligned}$$

If $\mu \neq 0$ the last term vanishes by the choice of $R = R_\mu$. If $\mu = 0$ it may be estimated using (5) and (77) as

$$Ch^{-3} \int_{d(v)>2R} |V(v)_-|^{5/2} dv \leq C\,.$$

Together with (88), (89), (102), and (103) this gives the proof of (10), and therefore finishes the proof of (7).

Step 3: Properties of the density.

We will now show that the density matrix γ in (101) satisfies the two requirements (8) and (9).

The density of γ is

$$\rho_\gamma(x) = \sum_{k=1}^{M} \theta_{r,k}(x)^2 \rho_k(x) + \int_{d(u)<2R+1} \varphi_u^2(x)\phi_+^2(x)\rho_u(x)\ell(u)^{-3}\,du\,, \tag{104}$$

where ρ_k for $k = 1, \ldots, M$ is the density of the density matrix γ_k and ρ_u for $u \in \mathbb{R}^3$ is the density for γ_u. We first control the 6/5-norm and the 1-norm of $\theta_{r,k}^2\rho_k$. If $\beta^{1/2}h^{-1} < 1/2$ we use the combined Daubechies-Lieb-Yau inequality (Theorem 16) with $\alpha = \beta^{1/2}h^{-1} \leq 1/2$, $\nu = 2z_k$, and $m = h^{-2}$ to obtain that

$$\begin{aligned} 0 \geq \mathrm{Tr}\big[\theta_{r,k}\gamma_k\theta_{r,k}(T_\beta(-\mathrm{i}h\nabla) - z_k|\hat{x} - r_k|^{-1})\big] \quad &\geq \quad \tfrac{1}{2}\,\mathrm{Tr}\big[\theta_{r,k}\gamma_k\theta_{r,k}T_\beta(-\mathrm{i}h\nabla)\big] \\ &\quad - Cz_k^{5/2}h^{-2} - Ch^{-3}z_k^{5/2}r^{1/2} - Cz_k^4h^2 \\ &\geq \quad \tfrac{1}{2}\,\mathrm{Tr}\big[\theta_{r,k}\gamma_k\theta_{r,k}T_\beta(-\mathrm{i}h\nabla)\big] - Ch^{-2}\delta^{-1/2}\,, \end{aligned}$$

where the constant C depends on z_k. Hence we have that

$$\mathrm{Tr}\big[T_\beta(-\mathrm{i}h\nabla)\theta_{r,k}\gamma_k\theta_{r,k}\big] \leq Ch^{-2}\delta^{-1/2} = Ch^{-5/2}\,. \tag{105}$$

Using (14) with $\alpha = \beta^{1/2}h^{-1} \leq 1$ and $m = h^{-2}$, (105) implies that

$$\begin{aligned} \int (\theta_{r,k}^2\rho_k)^{6/5} \quad &\leq \quad Ch^{-36/25}\left(\int_{h^2(\theta_{r,k}^2\rho_k)^{1/3}\leq\beta^{-1/2}h} h^2(\theta_{r,k}^2\rho_k)^{5/3}\right)^{18/25} r^{21/25} \\ &\quad + C\left(\int_{h^2(\theta_{r,k}^2\rho_k)^{1/3}>\beta^{-1/2}h} \beta^{-1/2}h(\theta_{r,k}^2\rho_k)^{4/3}\right)^{18/20} r^{3/10} \\ &\leq \quad Ch^{-36/25}h^{-9/5}h^{21/25} + Ch^{-9/4}h^{3/10} \leq Ch^{-12/5}\,, \end{aligned} \tag{106}$$

where we have used that $r = h$ and that h is bounded above by a constant. Likewise we find

$$\int \theta_{r,k}^2\rho_k \leq Ch^{-3/2}\,.$$

The case when $1/2 \leq \beta^{1/2}h^{-1} \leq 1$ is more complicated. We have to treat the region within the radius $r_- = h^2$ from the nucleus z_k differently. Let $\widetilde{\theta}_\pm(x) = \theta_\pm(|x - r_k|/h^2)$. Using the relativistic IMS formula (Theorem 13) and Theorem 14 with $\ell = h^2/2$, $m = h^{-2}$, $\alpha = \beta^{1/2}h^{-1}$, and $\Omega = \{|x - r_k| < 3h^2\}$ we find that

$$\begin{aligned} 0 &\geq \mathrm{Tr}\big[\theta_{r,k}\gamma_k\theta_{r,k}(T_\beta(-\mathrm{i}h\nabla) - z_k|\hat{x} - r_k|^{-1})\big] \\ &\geq \quad \mathrm{Tr}\big[\widetilde{\theta}_-\gamma_k\widetilde{\theta}_-(T_\beta(-\mathrm{i}h\nabla) - z_k|\hat{x} - r_k|^{-1} - Ch^{-2})\big] \\ &\qquad + \mathrm{Tr}\big[\theta_{r,k}\widetilde{\theta}_+\gamma_k\theta_{r,k}\widetilde{\theta}_+(T_\beta(-\mathrm{i}h\nabla) - z_k|\hat{x} - r_k|^{-1} - h^{-2}\chi_\Omega)\big] - Ch^{-2}\,. \end{aligned}$$

To treat the first term we use the inequality (see (21))

$$\sqrt{-\Delta} - \frac{2}{\pi|\hat{x}|} \geq A_s(-\Delta)^s - B_s\,,$$

which holds for all $0 \leq s < 1/2$ and $A_s, B_s > 0$ being constants depending only on s. Hence, using that h is bounded above by a constant and that $1 \leq \beta^{-1/2}h \leq 2$ we get

$$0 \geq \mathrm{Tr}\big[\widetilde{\theta}_-\gamma_k\widetilde{\theta}_-(T_\beta(-\mathrm{i}h\nabla) - z_k|\hat{x}-r_k|^{-1} - Ch^{-2})\big] \quad \geq \quad \mathrm{Tr}\big[\widetilde{\theta}_-\gamma_k\widetilde{\theta}_-(A_s(-\Delta)^s - C_sh^{-2})\big]\,.$$

We appeal to the standard (Daubechies)-Lieb-Thirring inequality

$$\mathrm{Tr}\big[(-\Delta)^s\widetilde{\theta}_-\gamma_k\widetilde{\theta}_-\big] \geq c\int(\widetilde{\theta}_-^2\rho_k)^{(3+2s)/3}\,,$$

which holds for all $s \in (0,3)$. We obtain that (with all constants depending on $0 < s < 1/2$)

$$\begin{aligned}\mathrm{Tr}\big[\widetilde{\theta}_-\gamma_k\widetilde{\theta}_-(T_\beta(-\mathrm{i}h\nabla) - z_k|\hat{x}-r_k|^{-1} - Ch^{-2})\big] \quad &\geq \quad c\int(\widetilde{\theta}_-^2\rho_k)^{(3+2s)/3} - Ch^{-2}\int(\widetilde{\theta}_-^2\rho_k)\\ &\geq \quad (c/2)\int(\widetilde{\theta}_-^2\rho_k)^{(3+2s)/3} - Ch^{(4s-3)/s}\,.\end{aligned}$$

Using the Daubechies inequality (Theorem 9) we find as above that

$$\begin{aligned}&\mathrm{Tr}\big[\theta_{r,k}\widetilde{\theta}_+\gamma_k\theta_{r,k}\widetilde{\theta}_+(T_\beta(-\mathrm{i}h\nabla) - z_k|\hat{x}-r_k|^{-1} - h^{-2}\chi_\Omega)\big]\\ &\quad\geq \quad c\,\mathrm{Tr}\big[\theta_{r,k}\widetilde{\theta}_+\gamma_k\theta_{r,k}\widetilde{\theta}_+T_\beta(-\mathrm{i}h\nabla)\big] - Ch^{-5/2}\,.\end{aligned}$$

By choosing s sufficiently close to $1/2$ and using that h is bounded by a constant we conclude that

$$0 \geq c\int(\widetilde{\theta}_-^2\rho_k)^{(3+2s)/3} + c\,\mathrm{Tr}\big[\theta_{r,k}\widetilde{\theta}_+\gamma_k\theta_{r,k}\widetilde{\theta}_+T_\beta(-\mathrm{i}h\nabla)\big] - Ch^{-5/2}\,.$$

As above it follows from this, choosing s sufficiently close to $1/2$, that we still have

$$\int(\theta_{r,k}^2\rho_k)^{6/5} \leq Ch^{-12/5}, \qquad \int\theta_{r,k}^2\rho_k \leq Ch^{-3/2}\,. \tag{107}$$

Using that $r = h$ and that from (5) $|V(x)| \leq Cd(x)^{-1}$ we also have

$$\int(h^{-3}\theta_{r,k}^2|V_-|^{3/2})^{6/5} \leq Ch^{-12/5}\,, \qquad \int h^{-3}\theta_{r,k}^2|V_-|^{3/2} \leq Ch^{-3/2}\,. \tag{108}$$

We move to the second term in (104). By the rescaled semi-classics (Theorem 23) we have on the support of $\varphi_u\phi_+$ that (for $f(u)$, see (95))

$$\Big|\rho_u(x) - 2^{1/2}(3\pi^2)^{-1}h^{-3}|V(x)_-|^{3/2}\Big| \leq Ch^{-2-1/10}f(u)^{21/10}\ell(u)^{-9/10} + Ch^{-2}|V(x)_-|^{3/2}\,,$$

where we have used that on the support of $\varphi_u\phi_+$ we have $|V(x)| \leq Cd(u)^{-1} \leq Cr^{-1} \leq Ch^{-1} \leq Ch\beta^{-1}$, since $d(u) \geq r/2$ if $\varphi_u\phi_+$ is non-vanishing. We moreover have on the support of $\varphi_u\phi_+$ that $|V(x)_-|^{3/2} \leq Cf(u)^3 \leq Cf(u)^{21/10}\ell(u)^{-9/10}$. For $r/2 < d(u) \leq 1$ this is because $\ell(u)^{-1} \geq d(u)^{-1} = f(u)^2 \geq f(u)$ (see (61)) and for $d(u) > 1$ we simply use that $\ell(u) \leq 1$ and $f(u) \leq 1$. Hence

$$\big\|\varphi_u^2\phi_+^2\big(\rho_\gamma - 2^{1/2}(3\pi^2)^{-1}h^{-3}|V_-|^{3/2}\big)\big\|_{6/5} \leq Ch^{-2-1/10}f(u)^{21/10}\ell(u)^{8/5}\,, \tag{109}$$

Using (101) and (102), we have that

$$
\begin{aligned}
&\big\|\rho_\gamma - 2^{1/2}(3\pi^2)^{-1}h^{-3}|V_-|^{3/2}\big\|_{6/5} \qquad (110)\\
&\leq \sum_{k=1}^{M}\big(\|\theta_{r,k}^2\rho_k\|_{6/5} + Ch^{-3}\|\theta_{r,k}^2|V_-|^{3/2}\|_{6/5}\big)\\
&\quad + \int_{d(u)<2R+1}\big\|\varphi_u^2\phi_+^2\big(\rho_u - 2^{1/2}(3\pi^2)^{-1}h^{-3}|V_-|^{3/2}\big)\big\|_{6/5}\ell(u)^{-3}du\\
&\quad + \int_{d(u)>2R+1} Ch^{-3}\big\|\varphi_u^2\phi_+^2|V_-|^{3/2}\big\|_{6/5}\ell(u)^{-3}du\,.
\end{aligned}
$$

The last term is non-zero only in the case $\mu = 0$ in which case it is easily seen by (6) and (77) to be bounded by $Ch^{-3/2}$. Thus, combining (106)–(109), (110) implies that

$$
\big\|\rho_\gamma - 2^{1/2}(3\pi^2)^{-1}h^{-3}|V_-|^{3/2}\big\|_{6/5} \leq Ch^{-2} + Ch^{-2-1/10}\int_{C^{-1}r<d(u)<2R+1} f(u)^{21/10}\ell(u)^{-7/5}du\,.
$$

The last integral is easily seen to be bounded and we arrive at (9).

To control the integral of the density we estimate

$$
\begin{aligned}
&\left|\int \rho_\gamma(x)\,dx - 2^{1/2}(3\pi^2)^{-1}h^{-3}\int |V(x)_-|^{3/2}\,dx\right|\\
&\leq \sum_{k=1}^{M}\big(\|\theta_{r,k}^2\rho_k\|_1 + Ch^{-3}\|\theta_{r,k}^2|V_-|^{3/2}\|_1\big)\\
&\quad + \int_{d(u)<2R+1}\left|\int \varphi_u^2\phi_+^2\big(\rho_u(x) - 2^{1/2}(3\pi^2)^{-1}h^{-3}|V(x)_-|^{3/2}\big)\,dx\right|\ell(u)^{-3}\,du\\
&\quad + \int_{d(u)>2R+1} Ch^{-3}\big\|\varphi_u^2\phi_+^2|V_-|^{3/2}\big\|_1\ell(u)^{-3}\,du\,.
\end{aligned}
$$

As before the last term is bounded by $Ch^{-3/2}$. For the middle term we again see from the rescaled semi-classics (Theorem 23) that

$$
\begin{aligned}
&\left|\int \varphi_u^2\phi_+^2\big(\rho_u(x) - 2^{1/2}(3\pi^2)^{-1}h^{-3}|V(x)_-|^{3/2}\big)dx\right|\\
&\leq Ch^{-2+1/5}f(u)^{9/5}\ell(u)^{9/5} + Ch^{-1}\int \varphi_u^2(x)\phi_+^2(x)|V(x)_-|^{5/2}dx\\
&\leq Ch^{-2+1/5}f(u)^{9/5}\ell(u)^{9/5} + Ch^{-1}f(u)^5\ell(u)^3\,,
\end{aligned}
$$

where we have used that $\beta \leq h^2$. The estimate (8) follows since both integrals

$$
\int f(u)^{9/5}\ell(u)^{9/5}\ell(u)^{-3}du \quad \text{and} \quad \int f(u)^5 du
$$

are bounded (recall that $f(u)$ is given in (95)). This finishes the proof of Theorem 4, except for the continuity of the function $\mathcal{S}$ from Lemma 25. We will need a lemma to prove this. This lemma also gives an alternative characterization of the function $\mathcal{S}$.

Lemma 27 (Scott-corrected pushed-up Hydrogen). *Let $\mathcal{S} : [0, 2/\pi] \to \mathbb{R}$ be the function from Lemma 25. Then there exists a constant $C > 0$ such that, for all $\alpha \in [0, 2/\pi]$*

and $\kappa \in (0,1]$,

$$\Big|\operatorname{Tr}\big[\sqrt{-\alpha^{-2}\Delta+\alpha^{-4}}-\alpha^{-2}-|\hat{x}|^{-1}+\kappa\big]_- \\ -(2\pi)^{-3}\int\big[\tfrac12 p^2-|v|^{-1}+\kappa\big]_-\,dpdv-\mathcal{S}(\alpha)\Big|\le C\kappa^{1/20}\,. \tag{111}$$

Here, as before, $\sqrt{-\alpha^{-2}\Delta+\alpha^{-4}}-\alpha^{-2}=-\Delta/2$, *when* $\alpha=0$.

Proof of Lemma 27. A simple rescaling, changing $x\to\kappa^{-1}\pi x/2$, gives

$$\operatorname{Tr}\big[\sqrt{-\alpha^{-2}\Delta+\alpha^{-4}}-\alpha^{-2}-|\hat{x}|^{-1}+\kappa\big]_-=\kappa\operatorname{Tr}\big[\sqrt{-\beta^{-1}h^2\Delta+\beta^{-2}}-\beta^{-1}-\frac{2}{\pi|\hat{x}|}+1\big]_-\,,$$

where $\beta=\kappa\alpha^2$ and $h=2\kappa^{1/2}/\pi$. We have $\beta\le h^2$.

The semi-classical integral may be rewritten in the same fashion,

$$(2\pi)^{-3}\int\big[\tfrac12 p^2-|v|^{-1}+\kappa\big]_-dpdv=\kappa\,(2\pi h)^{-3}\int\big[\tfrac12 p^2-\frac{2}{\pi|v|}+1\big]_-\,dpdv\,.$$

Since the potential $V(x)=\frac{2}{\pi|x|}-1$ satisfies the assumptions of Theorem 4 we see that there exists a constant $C>0$ such that

$$\Big|\operatorname{Tr}\big[\sqrt{-\beta^{-1}h^2\Delta+\beta^{-2}}-\beta^{-1}-\frac{2}{\pi|\hat{x}|}+1\big]_- \\ -\quad(2\pi h)^{-3}\int\big[\tfrac12 p^2-\frac{2}{\pi|v|}+1\big]_-\,dpdv-h^{-2}\frac{4}{\pi^2}\mathcal{S}(\alpha)\Big|\le C\,h^{-2+1/10}\,.$$

Using that $h=2\kappa^{1/2}/\pi$ gives (111). □

We can now, using the alternative characterization of the function $\mathcal{S}$ in Lemma 27, finish the proof of Theorem 4.

Step 4: Continuity of the function $\mathcal{S}$.

We recall that

$$T_\beta(p)=\begin{cases}\sqrt{\beta^{-1}p^2+\beta^{-2}}-\beta^{-1}\,, & \beta>0\\ \tfrac12 p^2\,, & \beta=0\end{cases}\,. \tag{112}$$

It suffices to prove continuity of

$$\operatorname{Tr}\big[T_{\alpha^2}(-\mathrm{i}\nabla)-|\hat{x}|^{-1}+\kappa\big]_-=\operatorname{Tr}\big[\sqrt{-\alpha^{-2}\Delta+\alpha^{-4}}-\alpha^{-2}-|\hat{x}|^{-1}+\kappa\big]_-$$

at all $\alpha_0\in[0,2/\pi]$, for any $\kappa\in(0,1]$ fixed. Then continuity of $\mathcal{S}$ follows from (111) by uniform convergence as $\kappa\to0$.

We first prove the continuity at $\alpha_0=0$.

Let $\chi_>=\chi_{|p|\ge\lambda}$, $\chi_<=\chi_{|p|\le\lambda}$ for some $\lambda>0$ to be chosen below. Note that $(\Gamma_1-\Gamma_2)(\Gamma_1-\Gamma_2)^*\ge0$ implies $\Gamma_1\Gamma_2^*+\Gamma_2\Gamma_1^*\le\Gamma_1\Gamma_1^*+\Gamma_2\Gamma_2^*$. Using this with $\Gamma_1=\varepsilon^{1/2}\chi_<|\hat{x}|^{-1/2}$, $\Gamma_2=\varepsilon^{-1/2}\chi_>|\hat{x}|^{-1/2}$ for some $\varepsilon>0$ which we choose later, we get the operator inequality

$$T_{\alpha^2}(\hat{p})-|\hat{x}|^{-1}+\kappa \\ \ge\quad\chi_>\big(T_{\alpha^2}(\hat{p})-(1+\varepsilon^{-1})|\hat{x}|^{-1}+\kappa\big)\chi_>+\chi_<\big(T_{\alpha^2}(\hat{p})-(1+\varepsilon)|\hat{x}|^{-1}+\kappa\big)\chi_<\,. \tag{113}$$

Here and in the sequel we write $T_{\alpha^2}(\hat{p})$ for the operator $T_{\alpha^2}(-\mathrm{i}\nabla)$ (and similarly for other operators). Since $T_{\alpha_1^2}\ge T_{\alpha_2^2}$ for $\alpha_1\le\alpha_2$, and $T_{\alpha^2}(p)\ge\alpha^{-1}|p|-\alpha^{-2}$, (113) implies that, if

$\alpha \in (0, A]$ for some $A > 0$, then for all $\varepsilon > 0$

$$\begin{aligned} T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa \quad &\geq \quad \chi_> \big(A^{-1}|\hat{p}| - A^{-2} - (1+\varepsilon^{-1})|\hat{x}|^{-1} + \kappa\big)\chi_> \\ &\qquad + \chi_< \big(T_{\alpha^2}(\hat{p}) - (1+\varepsilon)|\hat{x}|^{-1} + \kappa\big)\chi_< \,. \end{aligned} \tag{114}$$

Since $|\hat{p}| - 2/(\pi|\hat{x}|) \geq 0$, we have that

$$\frac{1}{2}A^{-1}|\hat{p}| - (1+\varepsilon^{-1})|\hat{x}|^{-1} \geq 0\,,$$

if $A \leq \varepsilon/(2\pi)$, and now assuming $\varepsilon \leq 1$. Furthermore, for $\lambda \geq 2A^{-1}$ we have that

$$\chi_> \big(\frac{1}{2}A^{-1}|\hat{p}| - A^{-2}\big)\chi_> \geq 0\,.$$

This implies that, if $\varepsilon \leq 1$, $\lambda \geq 2A^{-1}$, $\alpha \in (0, A]$ and $A \leq \varepsilon/(2\pi)$, then by (114)

$$T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa \quad \geq \quad \chi_< \big(T_{\alpha^2}(\hat{p}) - (1+\varepsilon)|\hat{x}|^{-1} + \kappa\big)\chi_< \,. \tag{115}$$

Since, by a Taylor-expansion, $T_{\alpha^2}(p) \geq T_0(p) - (\alpha p^2)^2/8$, and since $\chi_< = \chi_{|p|\leq\lambda}$, we have that, still for $\alpha \in (0, A]$,

$$T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa \geq \chi_< \big(T_0(\hat{p}) - \alpha^2\lambda^4/8 - (1+\varepsilon)|\hat{x}|^{-1} + \kappa\big)\chi_< \,. \tag{116}$$

Let

$$\gamma_{\alpha,\kappa} = \chi_{(-\infty,0]}\big(T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big)\,.$$

Then (116) and the fact that $T_0 \geq T_{\alpha^2}$ imply that, for $\alpha \in (0, A]$,

$$\begin{aligned} \mathrm{Tr}\big[T_0(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- \quad &\geq \quad \mathrm{Tr}\big[T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- = \mathrm{Tr}\big[\gamma_{\alpha,\kappa}\big(T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big)\big] \\ &\geq \quad \mathrm{Tr}\big[\gamma_{\alpha,\kappa}\chi_<\big(T_0(\hat{p}) - \alpha^2\lambda^4/8 - (1+\varepsilon)|\hat{x}|^{-1} + \kappa\big)\chi_<\big]\,. \end{aligned} \tag{117}$$

If $\kappa \in (0, 1]$, $\alpha \in (0, A]$, $\lambda \geq 2A^{-1}$, and $A \leq 1/(2\pi)$ we will show the a priori estimate

$$\mathrm{Tr}\big[\gamma_{\alpha,\kappa}\chi_<\big] \leq C\kappa^{-3/2} \qquad \text{and} \qquad \mathrm{Tr}\big[\gamma_{\alpha,\kappa}\chi_< \,|\hat{x}|^{-1}\chi_<\big] \leq C\kappa^{-1/2}\,. \tag{118}$$

The combined Daubechies-Lieb-Yau inequality (32) gives that for positive constants C_1, C_2 such that $\alpha \leq 2/(C_1\pi)$, we have

$$\begin{aligned} \mathrm{Tr}\big[T_{\alpha^2}(\hat{p}) - C_1|\hat{x}|^{-1} + C_2\kappa\big]_- \quad &\geq \quad -C\alpha^{1/2} - C\int_{|x|<C\kappa^{-1}} \big(|x|^{-1} + \kappa\big)^{5/2}\,dx \\ &\qquad - C\alpha^3 \int_{\alpha<|x|<C\kappa^{-1}} \big(|x|^{-1} + \kappa\big)^4\,dx \geq -C\kappa^{-1/2}\,. \end{aligned}$$

If $\alpha \in (0, A]$ and $A \leq 1/(2\pi)$ then $\alpha \leq 4/(5\pi)$ and hence we obtain from (115) with $\varepsilon = 1$ that

$$\begin{aligned} 0 \quad &\geq \quad \mathrm{Tr}\big[T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- = \mathrm{Tr}\big[\gamma_{\alpha,\kappa}\big(T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big)\big] \\ &\geq \quad \mathrm{Tr}\big[\gamma_{\alpha,\kappa}\chi_<\big(T_{\alpha^2}(\hat{p}) - 2|\hat{x}|^{-1} + \kappa\big)\chi_<\big] \\ &= \quad \mathrm{Tr}\big[\chi_<\gamma_{\alpha,\kappa}\chi_<\big(T_{\alpha^2}(\hat{p}) - \frac{5/2}{|\hat{x}|} + \frac{1}{2}\kappa\big)\big] + \frac{1}{2}\mathrm{Tr}\big[\gamma_{\alpha,\kappa}\chi_<|\hat{x}|^{-1}\chi_<\big] + \frac{\kappa}{2}\mathrm{Tr}\big[\gamma_{\alpha,\kappa}\chi_<\big] \\ &\geq \quad -C\kappa^{-1/2} + \frac{1}{2}\mathrm{Tr}\big[\gamma_{\alpha,\kappa}\chi_<|\hat{x}|^{-1}\chi_<\big] + \frac{\kappa}{2}\mathrm{Tr}\big[\gamma_{\alpha,\kappa}\chi_<\big]. \end{aligned}$$

This gives (118).

Choose $\lambda = 2A^{-1}$, $A = \epsilon/(2\pi)$. We combine (117) and (118) and use the variational principle to conclude that for $\alpha \in (0, \epsilon/(2\pi)]$, $\epsilon < 1$, and $\kappa \in (0, 1]$,

$$\begin{aligned}
\mathrm{Tr}\big[T_0(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- &\geq \mathrm{Tr}\big[T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- \\
&\geq \mathrm{Tr}\big[\big(\chi_< \gamma_{\alpha,\kappa} \chi_<\big)\big(T_0(\hat{p}) - |\hat{x}|^{-1} + \kappa\big)\big] - C\kappa^{-3/2}(\alpha^2\varepsilon^{-4} + \varepsilon) \\
&\geq \mathrm{Tr}\big[T_0(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- - C\kappa^{-3/2}(\alpha^2\varepsilon^{-4} + \varepsilon)\,.
\end{aligned}$$

Finally choose $\epsilon = \alpha^{2/5}$; then $\alpha \leq (2\pi)^{-5/3}$ implies that $\alpha \in (0, \epsilon/(2\pi)]$ and $\epsilon < 1$.

Therefore we have proved that for any $\alpha \leq (2\pi)^{-5/3}$ and $\kappa \in (0, 1]$,

$$\begin{aligned}
\mathrm{Tr}\big[T_0(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- &\geq \mathrm{Tr}\big[T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- \\
&\geq \mathrm{Tr}\big[T_0(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- - C\kappa^{-3/2}\alpha^{2/5}\,,
\end{aligned}$$

which proves continuity from the right of $\mathrm{Tr}\big[T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_-$ at $\alpha_0 = 0$ for any $\kappa \in (0, 1]$ fixed. (Notice that the above has not been optimized in κ.)

We now prove the continuity at any $\alpha_0 \in (0, 2/\pi)$. Note first that, for $0 < \alpha_1 \leq \alpha_2$,

$$T_{\alpha_1^2}(p) \geq T_{\alpha_2^2}(p) \geq (\alpha_2^{-1}\alpha_1)^2\, T_{\alpha_1^2}(p)\,. \tag{119}$$

Assume first that $\alpha > \alpha_0$, and let $\gamma_{\alpha,\kappa}$ be defined as above. Then, using (119) and the variational principle,

$$\begin{aligned}
\mathrm{Tr}[T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- &\leq \mathrm{Tr}\big[T_{\alpha_0^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- \leq \mathrm{Tr}\big[\gamma_{\alpha,\kappa}\big(T_{\alpha_0^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big)\big] \\
&\leq \mathrm{Tr}\big[\gamma_{\alpha,\kappa}\big(T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big)\big] + [(\alpha\alpha_0^{-1})^2 - 1]\,\mathrm{Tr}\big[\gamma_{\alpha,\kappa}T_{\alpha^2}(\hat{p})\big] \\
&= \mathrm{Tr}[T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- + [(\alpha\alpha_0^{-1})^2 - 1]\,\mathrm{Tr}\big[\gamma_{\alpha,\kappa}T_{\alpha^2}(\hat{p})\big]\,.
\end{aligned}$$

It remains to show that $[(\alpha\alpha_0^{-1})^2 - 1]\,\mathrm{Tr}\big[\gamma_{\alpha,\kappa}T_{\alpha^2}(\hat{p})\big] \to 0$ as $\alpha \to \alpha_0$. For this, it obviously suffices to show that $\mathrm{Tr}\big[\gamma_{\alpha,\kappa}T_{\alpha^2}(\hat{p})\big]$ is uniformly bounded for, say, $\alpha \in (\alpha_0, A]$ for some $A \in (\alpha_0, 2/\pi)$. But this follows as in the proof of (118). This proves continuity from the right of $\mathrm{Tr}\big[T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_-$ at $\alpha_0 \in (0, 2/\pi)$. To prove continuity from the left, assume $\alpha < \alpha_0$, and let $\gamma_{\alpha_0,\kappa}$ be defined as above. Then, by (119) and the variational principle,

$$\begin{aligned}
\mathrm{Tr}\big[T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- &\geq \mathrm{Tr}\big[T_{\alpha_0^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- = \mathrm{Tr}\big[\gamma_{\alpha_0,\kappa}\big(T_{\alpha_0^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big)\big] \\
&= \mathrm{Tr}\big[\gamma_{\alpha_0,\kappa}\big(T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big)\big] + \mathrm{Tr}\big[\gamma_{\alpha_0,\kappa}(T_{\alpha_0^2}(\hat{p}) - T_{\alpha^2}(\hat{p}))\big] \\
&\geq \mathrm{Tr}\big[T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- + [1 - (\alpha_0\alpha^{-1})^2]\,\mathrm{Tr}\big[\gamma_{\alpha_0,\kappa}T_{\alpha_0^2}(\hat{p})\big]\,.
\end{aligned}$$

As before, the last trace is finite by arguments as in the proof of (118) (since $\alpha_0 < 2/\pi$). This proves continuity from the left, and therefore, continuity, of $\mathrm{Tr}\big[T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_-$ at $\alpha_0 \in (0, 2/\pi)$.

Finally we prove the continuity at $\alpha_0 = 2/\pi$. Here, arguments as in the proof of (118) are no longer at our disposal. Therefore, let $\epsilon > 0$, and let $\gamma_{\alpha_0,\kappa}$ be defined as above, and choose $\phi_1, \ldots, \phi_N \in C_0^\infty(\mathbb{R}^3)$, $(\phi_i, \phi_j) = \delta_{i,j}$, such that

$$\begin{aligned}
&\mathrm{Tr}\big[\gamma_N\big(T_{\alpha_0^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big)\big] \\
&\quad\leq \mathrm{Tr}\big[\gamma_{\alpha_0,\kappa}\big(T_{\alpha_0^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big)\big] + \epsilon/2 = \mathrm{Tr}\big[T_{\alpha_0^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- + \epsilon/2\,,
\end{aligned} \tag{120}$$

for $\gamma_N(x, y) = \sum_{j=1}^N \phi_j(x)\overline{\phi_j(y)}$. This is possible since the operator is defined as the Friedrichs extension from $C_0^\infty(\mathbb{R}^3)$. (Here, both N and the ϕ_j's depend, of course, on ϵ).

Recall that γ_N is finite dimensional and $\phi_j \in C_0^\infty(\mathbb{R}^3)$. Using this, (119), and the variational principle gives that (for any $\alpha \in (\alpha_0/2, \alpha_0)$),

$$\begin{aligned}
\operatorname{Tr}\big[\gamma_N\big(T_{\alpha_0^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big)\big] &= \operatorname{Tr}\big[\gamma_N T_{\alpha_0^2}(\hat{p})\big] + \operatorname{Tr}\big[\gamma_N\big(-|\hat{x}|^{-1} + \kappa\big)\big] \\
&\geq \operatorname{Tr}\big[\gamma_N\big(T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big)\big] + [(\alpha_0^{-1}\alpha)^2 - 1]\operatorname{Tr}\big[\gamma_N T_{\alpha^2}(\hat{p})\big] \\
&\geq \operatorname{Tr}\big[T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- + [(\alpha_0^{-1}\alpha)^2 - 1]\operatorname{Tr}\big[\gamma_N T_{\alpha_0^2/2}(\hat{p})\big]\,. \qquad (121)
\end{aligned}$$

Choose now $\delta > 0$ such that

$$\alpha \in (\alpha_0 - \delta, \alpha_0) \cap (\alpha_0/2, \alpha_0) \quad \Rightarrow \quad [(\alpha_0^{-1}\alpha)^2 - 1]\operatorname{Tr}\big[\gamma_N T_{\alpha_0^2/2}(\hat{p})\big] > -\epsilon/2\,. \qquad (122)$$

Then, combining (120), (121), and (122) (and using (119) again) we have proved that, for all $\epsilon > 0$ there exists $0 < \delta < \alpha_0/2$ such that

$$\begin{aligned}
&\alpha \in (\alpha_0 - \delta, \alpha_0) \\
&\Rightarrow \quad \operatorname{Tr}\big[T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- \geq \operatorname{Tr}\big[T_{\alpha_0^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- \geq \operatorname{Tr}\big[T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_- - \epsilon\,.
\end{aligned}$$

This proves the continuity from the left of $\operatorname{Tr}\big[T_{\alpha^2}(\hat{p}) - |\hat{x}|^{-1} + \kappa\big]_-$ at $\alpha_0 = 2/\pi$, and therefore finishes the proof that $\mathcal{S} : [0, 2/\pi] \to \mathbb{R}$ is continuous.

This completes the proof of Theorem 4. □

5. Local relativistic semi-classical estimates using new coherent states

In this section we study the sum and the density of the negative eigenvalues of the localised Hamiltonian $\phi H_\beta \phi$, with ϕ compactly supported and $H_\beta = T_\beta(-\mathrm{i}h\nabla) + V(\hat{x})$. Here, T_β is given by (3), and V is a (sufficiently) regular potential (see below for details). For the most part we suppress the index β but all estimates, in particular the constants C, will be uniform in $\beta \in [0, 1]$.

We first recall the definition and the main properties of the coherent states (operators) introduced in [36], where all proofs can be found. These coherent states are denoted by $\mathcal{G}_{u,q}$. Let $1/a > h > 0$. The kernel of $\mathcal{G}_{u,q}$ is given by

$$\mathcal{G}_{u,q}(x, y) = (\pi h)^{-n/2} \mathrm{e}^{-a\left(\frac{x+y}{2} - u\right)^2 + \mathrm{i}q(x-y)/h - \frac{1}{4h^2 a}(x-y)^2}\,. \qquad (123)$$

A first important property of these operators is their completeness.

Lemma 28 (Completeness of new coherent states). *The coherent operators $\mathcal{G}_{u,q}$ satisfy*

$$\int \mathcal{G}_{u,q}^2 \frac{dq}{(2\pi h)^n} = G_b(\hat{x} - u)\,, \qquad \int \mathcal{G}_{u,q}^2 \frac{du}{(2\pi h)^n} = G_b(-\mathrm{i}h\nabla - q)\,, \qquad (124)$$

where $\hat{x}$ denotes the operator multiplication by the position variable x. Here $G_b(v) = (b/\pi)^{n/2}\mathrm{e}^{-bv^2}$ with $b = 2a/(1 + h^2a^2)$. Note that G_b has integral 1 and hence

$$\int \mathcal{G}_{u,q}^2 \frac{du dq}{(2\pi h)^n} = \mathbf{1}\,. \qquad (125)$$

We shall consider operators of the form

$$\int \mathcal{G}_{u,q}\, f(\widehat{A}_{u,q})\, \mathcal{G}_{u,q}\, du dq\,, \qquad (126)$$

where $f : \mathbb{R} \to \mathbb{R}$ is any polynomially bounded real function. As we shall see in the next theorem the integrand above is a trace class operator for each (u, q). The integral above is to be understood in the weak sense, i.e., as a quadratic form. We shall consider situations where the integral defines bounded or unbounded operators.

Theorem 29 (**Trace identity**). *Let $f:\mathbb{R}\to\mathbb{R}$ and $V:\mathbb{R}^n\to\mathbb{R}$ be polynomially bounded, real-valued measurable functions and let*

$$\hat{A} = B_0 + B_1\hat{x} - \mathrm{i}hB_2\nabla$$

be a first order self-adjoint differential operator[3] *with $B_0\in\mathbb{R}$, $B_{1,2}\in\mathbb{R}^n$. Then $\mathcal{G}_{u,q}\,f(\hat{A})\,\mathcal{G}_{u,q}\,V(\hat{x})$ is a trace class operator (when extended from $C_0^\infty(\mathbb{R}^n)$) and*

$$\begin{aligned}\mathrm{Tr}\big[\mathcal{G}_{u,q}\,f(\hat{A})\,\mathcal{G}_{u,q}\,V(\hat{x})\big] \;&=\; \int f(B_0+B_1v+B_2p)\,G_b(u-v)G_b(q-p)G_{(h^2b)^{-1}}(z)\\ &\qquad\qquad\times V(v+h^2ab(u-v)+z)\,dvdpdz\,.\end{aligned}$$

In particular, $\mathrm{Tr}\big[\mathcal{G}_{u,q}^2\big]=1$.

We shall also need the following extension of this theorem, where we however only give an estimate on the trace.

Theorem 30 (**Trace estimates**). *Let $f,\hat{A}$ be as in the previous theorem. Let moreover $\phi\in C^{n+4}(\mathbb{R}^n)$ be a bounded, real function with all derivatives up to order $n+4$ bounded, and let $V,F\in C^2(\mathbb{R}^n)$ be real functions with bounded second derivatives. Then, for $h<1$, $1<a<1/h$ and $b=2a/(1+h^2a^2)$ we have, with $\sigma(u,q)=F(q)+V(u)$, that*[4]

$$\begin{aligned}&\mathrm{Tr}\big[\mathcal{G}_{u,q}\,f(\hat{A})\,\mathcal{G}_{u,q}\,\phi(\hat{x})\big(F(-\mathrm{i}h\nabla)+V(\hat{x})\big)\phi(\hat{x})\big]\\ &\quad=\int f(B_0+B_1v+B_2p)\,G_b(u-v)G_b(q-p)\\ &\qquad\quad\times\Big[\big(\phi(v+h^2ab(u-v))^2+E_1(u,v)\big)\sigma(v+h^2ab(u-v),p+h^2ab(q-p))\\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad+E_2(u,v;q,p)\Big]\,dvdp\,,\end{aligned}$$

with $\|E_1\|_\infty,\|E_2\|_\infty\le Ch^2b$, where C depends only on

$$\sup_{|\nu|\le n+4}\|\partial^\nu\phi\|_\infty\,,\ \sup_{|\nu|=2}\|\partial^\nu V\|_\infty\,,\ \textit{and}\ \sup_{|\nu|=2}\|\partial^\nu F\|_\infty\,.$$

(Note that the assumption $1<a<1/h$ implies $1<b<1/h$.)

We will use the above theorem to prove an upper bound on the sum of eigenvalues of the operator $F(-\mathrm{i}h\nabla)+V(\hat{x})$, in the case when $F(q)=T_\beta(q)$ from (3) with $\beta\in[0,1]$ (equal to $\sqrt{\beta^{-1}q^2+\beta^{-2}}-\beta^{-1}$ for $\beta\in(0,1]$, and to $\frac12 q^2$ when $\beta=0$). This is done in Lemma 34 below by constructing a trial density matrix on the form (126).

To prove a lower bound on the sum of the negative eigenvalues one approximates the Hamiltonian $F(-\mathrm{i}h\nabla)+V(\hat{x})$ by an operator also represented on the form (126).

Theorem 31 (**Coherent states representation**). *Consider functions $F,V\in C^3(\mathbb{R}^n)$, for which all second and third derivatives are bounded. Let $\sigma(u,q)=F(q)+V(u)$, then for $a<1/h$ and $b=2a/(1+h^2a^2)$ we have the representation (as quadratic forms on $C_0^\infty(\mathbb{R}^n)$),*

$$F(-\mathrm{i}h\nabla)+V(\hat{x})=\int\mathcal{G}_{u,q}\widehat{H}_{u,q}\mathcal{G}_{u,q}\frac{dudq}{(2\pi h)^n}+\mathbf{E}\,,$$

with the operator-valued symbol

$$\widehat{H}_{u,q}=\sigma(u,q)+\tfrac{1}{4b}\Delta\sigma(u,q)+\partial_u\sigma(u,q)(\hat{x}-u)+\partial_q\sigma(u,q)(-ih\nabla-q)\,. \tag{127}$$

[3]The operator $\hat{A}$ is essentially self-adjoint on Schwartz functions on $\mathbb{R}^n$.

[4]The operator $\mathcal{G}_{u,q}\,f(\hat{A})\,\mathcal{G}_{u,q}\,\phi(\hat{x})\,(F(-\mathrm{i}h\nabla)+V(\hat{x}))\,\phi(\hat{x})$ is originally defined on, say, $C_0^\infty(\mathbb{R}^n)$, but it is part of the claim of the theorem that it extends to a trace class operator on all of $L^2(\mathbb{R}^n)$.

The error term, $\mathbf{E}$*, is a bounded operator with*

$$\|\mathbf{E}\| \le Cb^{-3/2} \sum_{|\nu|=3} \|\partial^\nu \sigma\|_\infty + Ch^2 b \sum_{|\nu|=2} \|\partial^\nu \sigma\|_\infty \,.$$

Let us recall our convention that $x_- = \min\{x, 0\}$ and that $\chi = \chi_{(-\infty,0]}$ denotes the characteristic function of $(-\infty, 0]$.

The next theorem is the main result of this section.

Theorem 32 (**Local relativistic semi-classics**)**.** *For* $n \ge 3$*, let* $\phi \in C_0^{n+4}(\mathbb{R}^n)$ *be supported in a ball* $B_1 \subset \mathbb{R}^n$ *of radius* 1 *and let* $V \in C^3(\overline{B_1})$ *be a real function. Let* $0 \le \beta \le 1$*,* $h > 0$*, and let* $\sigma_\beta(u,q) = T_\beta(q) + V(u)$ *and* $H_\beta = T_\beta(-\mathrm{i}h\nabla) + V(\hat{x})$ *with* $T_\beta(q) = \sqrt{\beta^{-1}q^2 + \beta^{-2}} - \beta^{-1}$ *for* $\beta \in (0,1]$ *and* $T_0(q) = \frac{1}{2}q^2$*.*

Then

$$\left|\mathrm{Tr}\left[\phi H_\beta \phi\right]_- - (2\pi h)^{-n} \int \phi(u)^2 \sigma_\beta(u,q)_-\, dudq\right| \le Ch^{-n+6/5} \,.$$

The constant $C > 0$ *here depends only on* $\|\phi\|_{C^{n+4}}$*,* $\|V\|_{C^3}$*,*[5] *and the dimension* n*, but not on* $\beta \in [0,1]$*.*

The important property for our method to work is that the second and third order derivatives of the kinetic energy function $T_\beta(q)$ are bounded uniformly in q and β. Thus the error term above is independent of $\beta \in [0,1]$, and in particular the same as for the non-relativistic case, $-h^2\Delta/2 + V$, which corresponds to the limit $\beta \to 0$. We prove upper and lower bounds and start with the lower bound.

Lemma 33 (**Lower bound on** $\mathrm{Tr}[\phi H_\beta \phi]_-$)**.** *Under the same conditions as in Theorem 32,*

$$\mathrm{Tr}[\phi H_\beta \phi]_- \ge (2\pi h)^{-n} \int \phi(u)^2 \sigma_\beta(u,q)_-\, dudq - Ch^{-n+6/5} \,.$$

The constant $C > 0$ *here depends only on* $\|\phi\|_{C^{n+4}}$*,* $\|V\|_{C^3}$*, and the dimension* n*, but not on* $\beta \in [0,1]$*.*

Proof. Since ϕ has support in the ball B_1 we may assume without loss of generality that $V \in C_0^3(\mathbb{R}^n)$ with the support in a ball B_2 of radius 2 and that the norm $\|V\|_{C^3}$ refers to the supremum over all of $\mathbb{R}^n$. We shall not explicitly follow how the error terms depend on $\|\phi\|_{C^{n+4}}$ and $\|V\|_{C^3}$. All constants denoted by C depend on $\|\phi\|_{C^{n+4}}$, $\|V\|_{C^3}$, and the dimension n but, in particular, not on β.

We use the Daubechies inequality (Theorem 9) to control various error estimates. Since $T_\beta(q) \ge T_1(q)$ for $\beta \in [0,1]$ we may use it with $\beta = 1$. Then, uniformly in $\beta \in [0,1]$,

$$\mathrm{Tr}[\phi H_\beta \phi]_- \ge C\|\phi\|_\infty^2 \int\limits_{u \in B_1} \sigma_1(u,q)_- \frac{dudq}{(2\pi h)^n} \ge -Ch^{-n} \,.$$

Consider some fixed $0 < \tau < 1$ (independent of h and β). If $h \ge \tau$ then we get that

$$\mathrm{Tr}[\phi H_\beta \phi]_- \ge \int \phi(u)^2 \sigma_\beta(u,q)_- \frac{dudq}{(2\pi h)^n} - C\tau^{-6/5} h^{-n+6/5} \,.$$

We are therefore left with considering $h < \tau$.

[5]We use the convention that $\|\psi\|_{C^p} = \sup_{|\nu| \le p} \|\partial^\nu \psi\|_\infty$.

If we now use the inequality $[x+y]_- \geq [x]_- + [y]_-$, which we will do frequently without further mentioning, and Theorem 31, we have that

$$\begin{aligned}\operatorname{Tr}[\phi H_\beta \phi]_- \quad &\geq \quad \operatorname{Tr}\Big[\int \phi\, \mathcal{G}_{u,q} \widehat{H}^{(\varepsilon)}_{u,q} \mathcal{G}_{u,q}\phi \, \frac{dudq}{(2\pi h)^n}\Big]_- \\ &\quad + \operatorname{Tr}\big[\phi\big(\varepsilon\sqrt{-\beta^{-1}h^2\Delta + \beta^{-2}} - \varepsilon\beta^{-1} - C(b^{-3/2}+h^2 b)\big)\phi\big]_- . \qquad (128)\end{aligned}$$

Here, $0 < \varepsilon < 1/2$ and

$$\widehat{H}^{(\varepsilon)}_{u,q} = \widetilde{\sigma}(u,q) + \tfrac{1}{4b}\Delta\widetilde{\sigma}(u,q) + \partial_u\widetilde{\sigma}(u,q)(\hat{x}-u) + \partial_q\widetilde{\sigma}(u,q)(-ih\nabla - q)$$

with $\widetilde{\sigma}(u,q) = (1-\varepsilon)T_\beta(q) + V(u)$. The second trace can be estimated from below using the Daubechies inequality (Theorem 9) with $\alpha = \beta^{1/2}h^{-1}$, $m = h^{-2}$. Then

$$\begin{aligned}&\operatorname{Tr}\big[\phi\big(\varepsilon\sqrt{-\beta^{-1}h^2\Delta+\beta^{-2}} - \varepsilon\beta^{-1} - C(b^{-3/2}+h^2b)\big)\phi\big]_- \\ &= \quad \varepsilon \operatorname{Tr}\big[\phi\big(\sqrt{-\beta^{-1}h^2\Delta+\beta^{-2}} - \beta^{-1} - C\varepsilon^{-1}(b^{-3/2}+h^2b)\big)\phi\big]_- \\ &\geq \quad -C\varepsilon h^{-n}\int_{B_1}\big(\varepsilon^{-1}(b^{-3/2}+h^2b)\big)^{1+n/2}\,dx \\ &\qquad - C\varepsilon\beta^{n/2}h^{-n}\int_{B_1}\big(\varepsilon^{-1}(b^{-3/2}+h^2b)\big)^{n}\,dx\,. \qquad (129)\end{aligned}$$

We shall eventually choose $\varepsilon = \frac{1}{4}(b^{-3/2}+h^2b)$. Note that then $\varepsilon < 1/2$, and that the bound in (129) is $-Ch^{-n}(b^{-3/2}+h^2b)$, uniformly for $\beta \in [0,1]$.

By bringing the negative part inside in (128) we obtain the lower bound,

$$\operatorname{Tr}[\phi H_\beta\phi]_- \geq \int \operatorname{Tr}\Big[\phi\,\mathcal{G}_{u,q}\big[\widehat{H}^{(\varepsilon)}_{u,q}\big]_-\mathcal{G}_{u,q}\phi\Big]\,\frac{dudq}{(2\pi h)^n} - Ch^{-n}(b^{-3/2}+h^2b)\,.$$

We first consider the integral over u outside the ball B_2 of radius 2, where $V = 0$. Using Theorem 29 (with $f(t) = [t]_-$, and V replaced by ϕ^2) and $\int\phi^2 \leq C$, we get that this part of the integral is

$$\begin{aligned}&(1-\varepsilon)\int\limits_{u\notin B_2}\Big[T_\beta(q) + (n+(n-1)\beta q^2)/[4b(1+\beta q^2)^{3/2}] + q\cdot(p-q)/\sqrt{1+\beta q^2}\,\Big]_- \\ &\qquad\qquad \times G_b(q-p)G_b(u-v)G_{(h^2b)^{-1}}(z)\phi(v+h^2ab(u-v)+z)^2\,dvdpdz\,\frac{dudq}{(2\pi h)^n} \\ &\geq \; (1-\varepsilon)\int\limits_{z\in B_1}\phi(z)^2\int\limits_{u\notin B_2} G_b(u-v)G_{(h^2b)^{-1}}(v+h^2ab(u-v)-z)\,dudvdz \\ &\qquad\qquad\qquad \times\int\big[T_\beta(q)+q\cdot(p-q)/\sqrt{1+\beta q^2}\,\big]_- G_b(q-p)\,\frac{dqdp}{(2\pi h)^n} \\ &= \; (1-\varepsilon)\int\limits_{z\in B_1}\phi(z)^2\int\limits_{(1-h^2ab)u\notin B_2-v} G_b(u)G_{(h^2b)^{-1}}(v-z)\,dudvdz \\ &\qquad\qquad\qquad\qquad \times\int\big[T_\beta(q)+q\cdot p/\sqrt{1+\beta q^2}\,\big]_- G_b(p)\,\frac{dqdp}{(2\pi h)^n}\,.\end{aligned}$$

The integration over u, v is obviously bounded by 1. In fact, the u-integration can be shown to be exponentially small, i.e., less than $C\,\mathrm{e}^{-Cb}$, but this will not be necessary.

The domain of integration for the variables q, p is contained in the set $\{(q,p)\,|\,|q| \le 2|p|\}$. Then,

$$\begin{aligned} &\int \left[T_\beta(q) + q\cdot p/\sqrt{1+\beta q^2}\,\right]_- G_b(p)\,dqdp \\ \geq \quad & -C \int\limits_{|q|<2|p|} \frac{|q||p|}{\sqrt{1+\beta q^2}} G_b(p)\,dqdp \geq -C\int |p|^{n+2} G_b(p)\,dp \;=\; -C\,b^{-(n+2)/2}\,. \end{aligned}$$

It follows that the integral over $u \notin B_2$ is bounded from below by $-Ch^{-n}b^{-3/2}$, since $b > 1$.

For the integral over $u \in B_2$ we use Theorem 29 as before. This time, expanding ϕ^2 to second order in z at the point $z = 0$ and using the crucial fact (which we shall use without mentioning later) that, for any $\lambda > 0$,

$$\int x_j\, G_\lambda(x)\,dx = 0\,, \qquad \int |x|^m\, G_\lambda(x)\,dx = C\,\lambda^{-m/2}\,, \tag{130}$$

implies that

$$\begin{aligned} \mathrm{Tr}[\phi H_\beta \phi]_- \geq \int\limits_{u\in B_2} &\left[\phi(v + h^2 ab(u-v))^2 + Ch^2 b\right] G_b(u-v) G_b(q-p) \\ &\times \left[H^{(\varepsilon)}_{u,q}(v,p)\right]_- \frac{dudq}{(2\pi h)^n} dvdp - Ch^{-n}(b^{-3/2} + h^2 b)\,, \end{aligned} \tag{131}$$

where

$$H^{(\varepsilon)}_{u,q}(v,p) = \widetilde{\sigma}(u,q) + \tfrac{1}{4b}\Delta\widetilde{\sigma}(u,q) + \partial_u\widetilde{\sigma}(u,q)(v-u) + \partial_q\widetilde{\sigma}(u,q)(p-q)\,.$$

The rest of the proof is simply an estimate of the integral in (131). This analysis is an elementary but tedious exercise in calculus. For the convenience of the reader it is given in detail in Appendix B below. □

Lemma 34 (Construction of a trial density matrix). *Under the same conditions as in Theorem 32 there exists a density matrix γ on $L^2(\mathbb{R}^n)$ such that*

$$\mathrm{Tr}\big[\phi(T_\beta(-ih\nabla) + V(\hat{x}))\phi\gamma\big] \leq \int \phi(u)^2 \sigma_\beta(u,q)_- \frac{dudq}{(2\pi h)^n} + Ch^{-n+6/5}\,. \tag{132}$$

Moreover, the density ρ_γ of γ satisfies

$$\Big|\rho_\gamma(x) - (2\pi h)^{-n}\omega_n\,|V_-|^{n/2}(2+\beta|V_-|)^{n/2}(x)\Big| \leq Ch^{-n+9/10}\,, \tag{133}$$

for (almost) all $x \in B_1$ and

$$\left|\int \phi(x)^2 \rho_\gamma(x)\,dx - (2\pi h)^{-n}\omega_n \int \phi(x)^2\,|V_-|^{n/2}(2+\beta|V_-|)^{n/2}(x)\,dx\right| \leq Ch^{-n+6/5}\,, \tag{134}$$

where ω_n is the volume of the unit ball B_1 in $\mathbb{R}^n$. The constants $C > 0$ in the above estimates depend only on n, $\|\phi\|_{C^{n+4}}$, and $\|V\|_{C^3}$, but not on $\beta \in [0,1]$.

It is convenient to introduce the function

$$\eta(t) = n\int_0^\infty \chi[T_\beta(p) + t]\,|p|^{n-1}\,d|p| = |t_-|^{n/2}(2+\beta|t_-|)^{n/2}\,. \tag{135}$$

(Recall that χ is the characteristic function of $\mathbb{R}_-$.)

Proof. We will occasionally drop the index β in H_β and σ_β. It is important to realize, however, that all estimates are uniform in β. We first note that since $T_1(p) \le T_\beta(p) \le T_0(p) = p^2/2$ we have that

$$|p| - C \le \sigma(v,p) \le \frac{1}{2}p^2 + C. \tag{136}$$

Let us start by choosing some fixed $0 < \tau < 1$. For $h \ge \tau$ and for some $C > 0$ we have by (136) that

$$\int \phi(u)^2 \sigma(u,q)_- \frac{du dq}{(2\pi h)^n} + C\tau^{-6/5} h^{-n+6/5} \ge 0\,,$$

and that for any $s > 0$,

$$(2\pi h)^{-n}\eta(V(x)) \le C\tau^{-s}h^{-n+s}\,.$$

If $h \ge \tau$ we may therefore use $\gamma = 0$, and $s = 9/10$ and $s = 6/5$ for (133) and (134), respectively. From now on we assume that $h < \tau$ and, if necessary, that τ is small enough depending only on ϕ and V. Also, as for the lower bound, we may assume that $V \in C_0^3(\mathbb{R}^n)$ with support in the ball $B_{3/2}$ concentric with B_1 and of radius $3/2$.

In analogy to the previous proof for the lower bound we define now for each (u,q) an operator $\hat{h}_{u,q}$ by

$$\hat{h}_{u,q} = \begin{cases} \sigma(u,q) + \frac{1}{4b}\Delta\sigma(u,q) + \nabla\sigma(u,q)\cdot(\hat{x} - u, -\mathrm{i}h\nabla - q) & \text{if } u \in B_2 \\ 0 & \text{if } u \notin B_2 \end{cases}.$$

The corresponding function is

$$h_{u,q}(v,p) = \begin{cases} \sigma(u,q) + \frac{1}{4b}\Delta\sigma(u,q) + \nabla\sigma(u,q)\cdot(v - u, p - q) & \text{if } u \in B_2 \\ 0 & \text{if } u \notin B_2 \end{cases}.$$

As for the lower bound we shall choose $a = h^{-4/5}$; then $a < h^{-1}$. In fact, we will assume that $(1 - h^2 ab) \ge 1/2$. Recall here that $b = 2a/(1 + h^2a^2)$ (i.e., in particular $a \le b \le 2a$).

Similar to (172) (for $\varepsilon = 0$) we have for $u \in B_2$ that

$$\begin{aligned}&\big|h_{u,q}(v,p) - \sigma(v,p) - \xi_{v,p}(u - v, q - p)\big| \\ &\qquad \le C|u - v|(b^{-1} + |u - v|^2) + C|q - p|(b^{-1} + |q - p|^2)\,,\end{aligned} \tag{137}$$

where

$$\xi_{v,p}(u,q) = \tfrac{1}{4b}\Delta\sigma(v,p) - \tfrac{1}{2}\sum_{i,j}\partial_i\partial_j T_\beta(p)q_iq_j - \tfrac{1}{2}\sum_{i,j}\partial_i\partial_j V(v)u_iu_j\,.$$

Recalling that χ is the characteristic function of $\mathbb{R}_-$ we define

$$\gamma = \int \mathcal{G}_{u,q}\,\chi\big[\hat{h}_{u,q}\big]\,\mathcal{G}_{u,q}\,\frac{du dq}{(2\pi h)^n}\,. \tag{138}$$

Since $\mathbf{0} \le \chi\big[\hat{h}_{u,q}\big] \le \mathbf{1}$ it follows from (125) that $\mathbf{0} \le \gamma \le \mathbf{1}$.

We now calculate $\mathrm{Tr}[\gamma\phi H_\beta \phi] = \mathrm{Tr}\big[\gamma\phi(T_\beta(-\mathrm{i}h\nabla) + V(\hat{x}))\phi\big]$. From Theorem 30 we have that

$$\begin{aligned}&\mathrm{Tr}\big[\gamma\phi(T_\beta(-\mathrm{i}h\nabla) + V(\hat{x}))\phi\big] \\ &\quad = \int \chi[h_{u,q}(v,p)]\,G_b(u - v)G_b(q - p)\Big[E_2(u,v;q,p) + \\ &\qquad \big(\phi(v + h^2ab(u - v))^2 + E_1(u,v)\big)\sigma(v + h^2ab(u - v), p + h^2ab(q - p))\Big]\,\frac{du dq}{(2\pi h)^n}dv dp\,,\end{aligned} \tag{139}$$

where E_1, E_2 are functions such that $\|E_1\|_\infty + \|E_2\|_\infty \le Ch^2 b$. The rest of the proof of (132) is a tedious, but elementary analysis of this integral. A detailed analysis is presented in Appendix B below.

It remains to estimate the density ρ_γ together with $\int \phi(x)^2 \rho_\gamma(x)\,dx$. By Theorem 29 and (138), γ is easily seen to be a trace class operator with density

$$\rho_\gamma(x) = \int \chi\big[h_{u+v,q+p}(v,p)\big] G_b(u) G_b(q) G_{(h^2b)^{-1}}(x - v - h^2 abu)\,dvdp\,\frac{dudq}{(2\pi h)^n}\,. \tag{140}$$

The proof of (133) and (134) again relies on a detailed analysis of this integral. As for the estimate on the energy above this analysis is an exercise in calculus. Although it is still elementary this analysis is more complicated than in the case of the energy. For the convenience of the reader the analysis is given in detail in Appendix B below. ☐

Appendix A. Various Proofs

In this appendix we collect proofs of various results mentioned in Section 2.

Proof of Theorem 11 (**Operator inequality critical Hydrogen**). Let $f \in \mathcal{S}(\mathbb{R}^3)$ and $t > 0$ (to be chosen below). By Schwarz' inequality,

$$\begin{aligned}\frac{2}{\pi}\int_{\mathbb{R}^3} \frac{|f(x)|^2}{|x|}\,dx &= \frac{1}{\pi^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\overline{\hat f(p)}\hat f(q)}{|p-q|^2}\Big(\frac{|p|^2+|p|^t}{|q|^2+|q|^t}\Big)^{1/2}\Big(\frac{|q|^2+|q|^t}{|p|^2+|p|^t}\Big)^{1/2} dpdq \\ &\le \frac{1}{\pi^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|\hat f(p)|^2}{|p-q|^2}\,\frac{|p|^2+|p|^t}{|q|^2+|q|^t}\,dpdq\,. \end{aligned} \tag{141}$$

We first compute the integral in q. Since $(|q|^2+|q|^t)^{-1} \le |q|^{-2} - |q|^{t-4} + |q|^{2t-6}$ we get

$$\int_{\mathbb{R}^3} \frac{1}{|p-q|^2}\,\frac{1}{|q|^2+|q|^t}\,dq \le \int_{\mathbb{R}^3} \frac{1}{|p-q|^2}\,(|q|^{-2} - |q|^{t-4} + |q|)^{2t-6}\,dq\,.$$

Note [19, 5.10 (3)] that, for $0 < \tau, \sigma < n$, with $0 < \tau + \sigma < n$,

$$\int_{\mathbb{R}^n} |y-z|^{\tau-n}|z|^{\sigma-n}\,dz = \frac{c_{n-\tau-\sigma}c_\tau c_\sigma}{c_{\tau+\sigma}c_{n-\tau}c_{n-\sigma}}\,|y|^{\tau+\sigma-n}\,, \tag{142}$$

where $c_\tau = \pi^{-\tau/2}\Gamma(\tau/2)$. In particular, if $n = 3$, then

$$\int_{\mathbb{R}^3} |y-z|^{-2}|z|^{-r}\,dz = k_r\,|y|^{1-r} \text{ for } r \in (1,3)\,, \tag{143}$$

with

$$k_r = \pi^2 \frac{\Gamma\big(\frac{r-1}{2}\big)\Gamma\big(\frac{3-r}{2}\big)}{\Gamma\big(\frac{4-r}{2}\big)\Gamma\big(\frac{r}{2}\big)}\,. \tag{144}$$

It follows that, for $3 < 2t < 5$,

$$\begin{aligned}\int_{\mathbb{R}^3} \frac{1}{|p-q|^2}\,\frac{|p|^2+|p|^t}{|q|^2+|q|^t}\,dq &\le k_2\,|p| + (k_2 - k_{4-t})\,|p|^{t-1} \\ &\quad + \big(k_{6-2t} - k_{4-t}\big)\,|p|^{2t-3} + k_{6-2t}\,|p|^{3t-5}\,. \end{aligned} \tag{145}$$

We see from (144) that k is symmetric with respect to $r = 2$. Using $\Gamma(1+z) = z\Gamma(z)$ in the denominator in (144) with $z = 1 - r/2$ and the relation $\Gamma(z)\Gamma(1-z) = \pi/\sin(\pi z)$ (for $0 < z < 1$) in the denominator and numerator we obtain

$$k_r = -\pi^2\,\frac{\tan(\pi r/2)}{1 - r/2}\,,$$

which shows that k is decreasing on $(1,2)$ and increasing on $(2,3)$.

Hence from (145), choosing further $t > 5/3$, we find, for positive constants $A_{(t-1)/2}$, $B_{(t-1)/2}$, that

$$\int_{\mathbb{R}^3} \frac{1}{|p-q|^2} \frac{|p|^2+|p|^t}{|q|^2+|q|^t}\, dq \quad \leq \quad k_2\,|p| - \pi^3 A_{(t-1)/2}|p|^{t-1} + \pi^3 B_{(t-1)/2}\,. \tag{146}$$

Since $k_2 = \pi^3$, this and (141) implies that

$$\frac{2}{\pi}\int_{\mathbb{R}^3} \frac{|f(x)|^2}{|x|}\, dx \quad \leq \quad \int_{\mathbb{R}^3} |\hat{f}(p)|\big(|p| - A_{(t-1)/2}|p|^{t-1} + B_{(t-1)/2}\big)\, dp\,, \tag{147}$$

which implies the operator inequality, for all $t \in (5/3, 2)$,

$$\sqrt{-\Delta} - \frac{2}{\pi|\hat{x}|} \quad \geq \quad A_{(t-1)/2}(-\Delta)^{(t-1)/2} - B_{(t-1)/2}\,. \tag{148}$$

Choosing $t = 2s+1$ proves (21) for $s \in (1/3, 1/2)$. For $s \in [0, 1/3]$, (21) follows from the existence of positive constants $A_{(\tau-1)/2}$, $B_{(\tau-1)/2}$, given $\tau \in [1, 5/3], t \in (5/3, 2)$ and positive constants $A_{(t-1)/2}, B_{(t-1)/2}$, such that

$$A_{(t-1)/2}|p|^{t-1} - B_{(t-1)/2} \quad \geq \quad A_{(\tau-1)/2}|p|^{\tau-1} - A_{(\tau-1)/2}\,.$$

$\square$

Integral representation for the relativistic kinetic energy. We shall here give a self-contained presentation of the integral formulas for the relativistic kinetic energy. The relativistc kinetic energy will be given in terms of the modified Bessel functions of the second kind, K_ν. To identify the modified Bessel functions we use that [1, 9.6.23]

$$K_0(t) = \int_1^\infty \frac{\mathrm{e}^{-wt}}{\sqrt{w^2-1}}\, dw\,, \quad t > 0\,, \tag{149}$$

and the recursion relation [1, 9.6.28]

$$K_{\nu+1}(t) = -t^\nu \frac{d}{dt}(t^{-\nu}K_\nu(t))\,, \quad t > 0\,. \tag{150}$$

We emphasise that we use these properties only as *definitions* of the Bessel functions, and derive all other properties of these functions that we need. Note that $K_\nu : \mathbb{R}_+ \to \mathbb{R}$ are smooth functions.

Consider the function $G_n^m \in L^1(\mathbb{R}^n)$ (the Yukawa potential) whose Fourier transform is

$$\widehat{G_n^m}(\xi) = (2\pi)^{-n/2}(|\xi|^2 + m^2)^{-1}\,.$$

Using that $v^{-1} = \int_0^\infty \mathrm{e}^{-uv}\, du$ we get from the Fourier transform of Gaussian functions the following integral representation for G,

$$G_n^m(z) = \int_0^\infty (4\pi u)^{-n/2}\mathrm{e}^{-m^2u - |z|^2/(4u)}\, du\,. \tag{151}$$

It follows from this that G is non-negative, smooth for $z \neq 0$, and indeed in $L^1(\mathbb{R}^n)$.

For odd n the above integral can be explicitly calculated. For even n it is as we shall now see expressible as a modified Bessel function K_ν of integer order ν. By a simple change of variables ($2w = v + v^{-1}$ with $v = 2mu/|z|$) in the integral (149) we see from (151) that $G_2^m(z) = (2\pi)^{-1}K_0(m|z|)$. From the recursion formula (150) we then find inductively that for even n

$$G_n^m(z) = m^{(n-2)/2}(2\pi)^{-n/2}|z|^{-(n-2)/2}K_{(n-2)/2}(m|z|)\,. \tag{152}$$

In fact, the same formula holds for all n, but we do not wish to discuss the modified Bessel functions of fractional order (one could simply take this formula as their definition).

Lemma 35. *The heat kernel for the operator* $\sqrt{-\Delta+m^2}$ *on* $L^2(\mathbb{R}^n)$ *is given by*

$$\begin{aligned}
&\exp(-t\sqrt{-\Delta+m^2})(x,y)\\
&= -2\partial_t G^m_{n+1}(x-y,t)\\
&= 2\left(\frac{m}{2\pi}\right)^{(n+1)/2}\frac{t}{(|x-y|^2+t^2)^{(n+1)/4}}K_{(n+1)/2}(m(|x-y|^2+t^2)^{1/2})
\end{aligned}$$

for $t>0$.

Proof. It suffices to show that the two tempered distributions on $\mathbb{R}^{n+1}$,

$$\frac{t}{|t|}\exp(-|t|\sqrt{-\Delta+m^2})(x,0) \quad\text{and}\quad -2\partial_t G^m_{n+1}(x,t)\,,$$

have the same Fourier transform. The Fourier transform as a function of $\xi=(p,s)$ with $p\in\mathbb{R}^n$ and $s\in\mathbb{R}$ of the first distribution is

$$(2\pi)^{-(n+1)/2}\Big(-\int_{-\infty}^0 \mathrm{e}^{-its+t\sqrt{p^2+m^2}}\,dt+\int_0^\infty \mathrm{e}^{-its-t\sqrt{p^2+m^2}}\,dt\Big)=\frac{-2\mathrm{i}s(2\pi)^{-(n+1)/2}}{|p|^2+s^2+m^2}\,.$$

The Fourier transform of the second distribution above is

$$-2\mathrm{i}s\,\widehat{G}^m_{n+1}(p,s)=\frac{-2\mathrm{i}s(2\pi)^{-(n+1)/2}}{|p|^2+s^2+m^2}\,.$$

The last identity in the lemma follows from (150) and (152). □

If we set $x=y$ in the above lemma we find the following integral formula for the modified Bessel function

$$K_{(n+1)/2}(t)=\frac{1}{2}\left(\frac{t}{2\pi}\right)^{(n-1)/2}\int_{\mathbb{R}^n}\mathrm{e}^{-t\sqrt{p^2+1}}\,dp\,,\quad t>0\,.$$

For $n=3$ this simplifies to

$$K_2(t)=t\int_0^\infty \mathrm{e}^{-t\sqrt{s^2+1}}s^2\,ds \tag{153}$$

from which we immediately get the estimate

$$K_2(t)\le Ct^{-2}\mathrm{e}^{-t/2}\,. \tag{154}$$

Proof of Theorem 13 (**Relativistic IMS formula**). By scaling, it suffices to prove the statement for $\alpha=1$. We start from the identity

$$\big(f,(\sqrt{-\Delta+m^2}-m)f\big)=\int|f(x)-f(y)|^2F(x-y)\,dxdy$$

with

$$F(x-y)=\frac{m^2}{4\pi^2}\,\frac{K_2(m|x-y|)}{|x-y|^2}\,, \tag{155}$$

where K_2 is the modified Bessel function of second order defined above (see (149)–(150)). The identity follows from Lemma 35 (for a proof, see [19, 7.12]). Then,

$$
\begin{aligned}
&\big(f, (\sqrt{-\Delta+m^2}-m)f\big)\\
&= \int |f(x)-f(y)|^2 F(x-y)\,dxdy\\
&= \int\int_{\mathcal{M}} \big[\theta_u(x)^2|f(x)|^2+\theta_u(y)^2|f(y)|^2\big]\,F(x-y)\,d\mu(u)dxdy\\
&\quad + \int\int_{\mathcal{M}} \big[-\tfrac{1}{2}(\theta_u(x)^2+\theta_u(y)^2)+\theta_u(x)\theta_u(y)-\theta_u(x)\theta_u(y)\big]\\
&\qquad\qquad \times \big[\,\overline{f(x)}f(y)+f(x)\overline{f(y)}\,\big]\,F(x-y)\,d\mu(u)dxdy\\
&= \int\int_{\mathcal{M}} |\theta_u(x)f(x)-\theta_u(y)f(y)|^2 F(x-y)\,d\mu(x)dxdy\\
&\quad + \int\int_{\mathcal{M}} \big[-\tfrac{1}{2}(\theta_u(x)^2+\theta_u(y)^2)+\theta_u(x)\theta_u(y)\big]\\
&\qquad\qquad \times \big[\,\overline{f(x)}f(y)+f(x)\overline{f(y)}\,\big]\,F(x-y)\,d\mu(u)dxdy\\
&= \int_{\mathcal{M}} \big(\theta_u f, (\sqrt{-\Delta+m^2}-m)\theta_u f\big)\,d\mu(u)\\
&\quad - \int\int_{\mathcal{M}} \big(\theta_u(x)-\theta_u(y)\big)^2 f(x)\overline{f(y)}F(x-y)\,d\mu(u)dxdy\,.
\end{aligned}
$$

This proves (23) with L given by (24)–(25). We now show that $\|L_{\theta_u}\| \le Cm^{-1}\|\nabla\theta_u\|_\infty^2$ for fixed u. By (25), Young's inequality, and (154),

$$
\begin{aligned}
\big|(f, L_{\theta_u} f)\big| &\le \frac{m^2}{4\pi^2}\|\nabla\theta_u\|_\infty^2 \int |f(x)|\,|f(y)|\,K_2(m|x-y|)\,dxdy\\
&\le C\,m^2\|\nabla\theta_u\|_\infty^2\|f\|_2^2\int_0^\infty t^2K_2(mt)\,dt\\
&= C\,m^{-1}\|\nabla\theta_u\|_\infty^2\|f\|_2^2\,.
\end{aligned}
\tag{156}
$$

This proves that L_{θ_u} is a bounded operator. □

Proof of Theorem 14 (**Localisation error**). Again, by scaling, it suffices to prove the statement for $\alpha = 1$. With χ_Ω the characteristic function of Ω (and $L \equiv L_\theta$) we have from the representation (25) of L, since θ is constant on Ω^c, that

$$
L = \chi_\Omega L\chi_\Omega + (1-\chi_\Omega)L\chi_\Omega + \chi_\Omega L(1-\chi_\Omega). \tag{157}
$$

If Γ_1, Γ_2 are bounded operators, then $(\Gamma_1-\Gamma_2)(\Gamma_1-\Gamma_2)^* \ge 0$ implies that $\Gamma_1\Gamma_2^*+\Gamma_2\Gamma_1^* \le \Gamma_1\Gamma_1^*+\Gamma_2\Gamma_2^*$. Using this with $\Gamma_1 = \varepsilon^{1/2}\chi_\Omega, \Gamma_2 = \varepsilon^{-1/2}(1-\chi_\Omega)L$ for some $\varepsilon > 0$ which we choose later, we get

$$
L \le \chi_\Omega L\chi_\Omega + \varepsilon\chi_\Omega + \varepsilon^{-1}(1-\chi_\Omega)L^2(1-\chi_\Omega)\,. \tag{158}
$$

To bound the first term on the right side recall that $\|L\| \le Cm^{-1}\|\nabla\theta\|_\infty^2$ (see (156)).

Let us now look at the third term in (158). Since θ is constant on Ω^c and $\mathrm{dist}(\Omega^c, \mathrm{supp}\,\nabla\theta) \geq \ell$, using (25) gives

$$\begin{aligned}\mathrm{Tr}\big[(1-\chi_\Omega)L^2(1-\chi_\Omega)\big] &= \int_{x\in\Omega^c, y\in\Omega, |x-y|>\ell} L(x,y)^2\,dxdy \\ &\leq Cm^4\|\nabla\theta\|_\infty^4 \int_{x\in\Omega^c, y\in\Omega, |x-y|>\ell} K_2(m|x-y|)^2\,dxdy\,.\end{aligned}$$

Using (154),

$$\begin{aligned}&\int_{x\in\Omega^c, y\in\Omega, |x-y|>\ell} K_2(m|x-y|)^2\,dxdy \\ &\qquad\leq C\mathrm{e}^{-m\ell}\int_{x\in\Omega^c, y\in\Omega, |x-y|>\ell} (m|x-y|)^{-4}\,dxdy \\ &\qquad= C\mathrm{e}^{-m\ell}|\Omega|\int_\ell^\infty (mt)^{-4}t^2\,dt = Cm^{-3}(m\ell)^{-1}\mathrm{e}^{-m\ell}|\Omega|\,.\end{aligned}$$

This gives the bound

$$\mathrm{Tr}\big[(1-\chi_\Omega)L^2(1-\chi_\Omega)\big] \leq C\ell^{-1}\|\nabla\theta\|_\infty^4\mathrm{e}^{-m\ell}|\Omega|\,.$$

Finally, we choose $\varepsilon = m^{-1}\|\nabla\theta\|_\infty^2$. Then by the above the two first terms in (158) are bounded by $Cm^{-1}\|\nabla\theta\|_\infty^2\chi_\Omega$, and the trace of the third term (which we denote Q_θ) is bounded by $Cm\ell^{-1}\mathrm{e}^{-m\ell}\|\nabla\theta\|_\infty^2|\Omega|$. □

For the proof of the combined Daubechies-Lieb-Yau inequality (Theorem 16) we need the following inequality [5].

Lemma 36. *For $f \in \mathcal{S}(\mathbb{R}^3)$,*

$$\int_{\mathbb{R}^3} \frac{\mathrm{e}^{-m^2\pi^{-1}|x|^2}}{|x|}|f(x)|^2\,dx \leq \frac{\pi}{2}\frac{1}{\sqrt{2}-1}\big(f, (\sqrt{-\Delta+m^2}-m)f\big)\,. \tag{159}$$

Proof. Let $\mu = m^2\pi^{-1}$. Then

$$I = \int_{\mathbb{R}^3}\frac{\mathrm{e}^{-\mu|x|^2}}{|x|}|f(x)|^2\,dx = \frac{1}{2\pi^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\overline{\hat{f}(p_1)}\frac{1}{|p_1-p_2|^2}\hat{g}(p_2)\,dp_1dp_2\,,$$

with $g(x) = f(x)\mathrm{e}^{-\mu|x|^2}$. Writing $\hat{g}(p_2)$ explicitly as the convolution with the Fourier transform of $\mathrm{e}^{-\mu|x|^2}$ and then applying the Schwarz inequality we get that

$$I \leq \frac{1}{16\pi^2(\pi\mu)^{3/2}}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|\hat{f}(p_1)|^2\mathrm{e}^{-|q|^2/(4\mu)}}{|p_2-p_1-q|^2}\frac{|p_1|^2}{|p_2|^2}\,dp_1dp_2dq\,.$$

Since [19, 5.10 (3)]

$$\int_{\mathbb{R}^3}\frac{1}{|p_2-p_1-q|^2}\frac{1}{|p_2|^2}\,dp_2 = \frac{\pi^3}{|p_1-q|}\,,$$

we have

$$I \leq \frac{1}{16\pi^{1/2}\mu^{3/2}}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|\hat{f}(p_1)|^2\mathrm{e}^{-|q|^2/(4\mu)}}{|p_1-q|}|p_1|^2\,dp_1dq\,.$$

By Newton's theorem [19, 9.7 (5)],

$$
\begin{aligned}
\int_{\mathbb{R}^3} \frac{\mathrm{e}^{-|q|^2/(4\mu)}}{|p_1-q|}\,dq &= \frac{1}{|p_1|}\int_{|q|<|p_1|} \mathrm{e}^{-|q|^2/(4\mu)}\,dq + \int_{|q|>|p_1|} \frac{\mathrm{e}^{-|q|^2/(4\mu)}}{|q|}\,dq \\
&= \frac{8\pi\mu}{|p_1|}\int_0^{|p_1|} \mathrm{e}^{-r^2/(4\mu)}\,dr \le 8\pi\mu \min\big\{1, \frac{(\pi\mu)^{1/2}}{|p_1|}\big\}\,.
\end{aligned}
$$

Substituting $\mu = m^2\pi^{-1}$ we find that

$$
I \le \frac{\pi}{2m}\int_{\mathbb{R}^3} |\hat f(p_1)|^2 \min\{|p_1|^2, m|p_1|\}\,dp_1\,,
$$

from which the claim follows since $\sqrt{t^2+1}-1 \ge (\sqrt{2}-1)\min\{t^2,t\}$ for $t\ge 0$. $\square$

Proof of Theorem 16 (**Combined Daubechies-Lieb-Yau**). We may assume that $W(x)\le 0$ otherwise we simply replace W by W_-.

Assume first that $\nu\alpha \le 3/(16\pi M)$. By the Daubechies inequality (17),

$$
\begin{aligned}
&\mathrm{Tr}\big[\sqrt{-\alpha^{-2}\Delta + m^2\alpha^{-4}} - m\alpha^{-2} + W(\hat x)\big]_- \\
&\ge \tfrac12 \mathrm{Tr}\big[\sqrt{-\alpha^{-2}\Delta + m^2\alpha^{-4}} - m\alpha^{-2} + 2W\chi_{\{d_{\mathbf{R}}(x)<\alpha m^{-1}\}}\big]_- \qquad (160)\\
&\quad - Cm^{3/2}\int_{d_{\mathbf{R}}(x)>\alpha m^{-1}} |W(x)|^{5/2}\,dx - C\alpha^3 \int_{d_{\mathbf{R}}(x)>\alpha m^{-1}} |W(x)|^4\,dx\,.
\end{aligned}
$$

The assumption on the positions of the nuclei implies that $\chi_{\{d_{\mathbf{R}}(x)<\alpha m^{-1}\}} = \sum_{j=1}^M \chi_{\{|x-R_j|<\alpha m^{-1}\}}$, and so, using the assumption on W, we obtain

$$
\begin{aligned}
&\mathrm{Tr}\big[\sqrt{-\alpha^{-2}\Delta + m^2\alpha^{-4}} - m\alpha^{-2} + 2W\chi_{\{d_{\mathbf{R}}(x)<\alpha m^{-1}\}}\big]_- \\
&\ge \frac{1}{M}\sum_{j=1}^M \mathrm{Tr}\big[\sqrt{-\alpha^{-2}\Delta + m^2\alpha^{-4}} - m\alpha^{-2} - \big(\frac{2\nu M}{|\hat x - R_j|} + C\nu M m\alpha^{-1}\big)\chi_{\{|x-R_j|<\alpha m^{-1}\}}\big]_- \\
&= \mathrm{Tr}\big[\sqrt{-\alpha^{-2}\Delta + m^2\alpha^{-4}} - m\alpha^{-2} - \big(2\nu M|\hat x|^{-1} + C\nu M m\alpha^{-1}\big)\chi_{\{|x|<\alpha m^{-1}\}}\big]_-\,. \qquad (161)
\end{aligned}
$$

The last equality follows from the translation invariance of $-\Delta$. By scaling,

$$
\begin{aligned}
&\mathrm{Tr}\big[\sqrt{-\alpha^{-2}\Delta + m^2\alpha^{-4}} - m\alpha^{-2} - \big(2\nu M|\hat x|^{-1} + C\nu M m\alpha^{-1}\big)\chi_{\{|x|<\alpha m^{-1}\}}\big]_- \\
&= \alpha^{-2}\,\mathrm{Tr}\big[\sqrt{-\Delta+m^2} - m - \big(\gamma|\hat x|^{-1} + C\gamma m\big)\chi_{\{|x|<m^{-1}\}}\big]_-\,, \qquad (162)
\end{aligned}
$$

with $\gamma = 2M\nu\alpha \le 3/(8\pi)$. Using Lemma 36 and the Daubechies inequality, we get that

$$
\begin{aligned}
&\mathrm{Tr}\big[\sqrt{-\Delta+m^2} - m - \big(\gamma|\hat x|^{-1} + C\gamma m\big)\chi_{\{|x|<m^{-1}\}}\big]_- \\
&\ge \big(1-\tfrac{4\pi}{3}\gamma\big)\,\mathrm{Tr}\big[\sqrt{-\Delta+m^2} - m - \gamma\big(1-\tfrac{4\pi}{3}\gamma\big)^{-1}\big(\frac{1-\mathrm{e}^{-m^2\pi^{-1}|\hat x|^2}}{|\hat x|} + Cm\big)\chi_{\{|x|<m^{-1}\}}\big]_- \\
&\ge -C\gamma^{5/2}m^{3/2}\int_{|x|<m^{-1}} \big(|x|^{-1}+m\big)^{5/2}\,dx - C\gamma^4\int_{|x|<m^{-1}} \Big(\frac{1-\mathrm{e}^{-m^2\pi^{-1}|x|^2}}{|x|} + m\Big)^4\,dx\,,
\end{aligned}
$$

where we have used that $\sqrt{2}-1\ge 3/8$ and $\gamma \le 3/(8\pi)$.

Note that

$$
\int_{|x|<m^{-1}} \big(|x|^{-1}+m\big)^{5/2}\,dx \le Cm^{-1/2}\,, \qquad \int_{|x|<m^{-1}} \Big(\frac{1-\mathrm{e}^{-m^2\pi^{-1}|x|^2}}{|x|} + m\Big)^4\,dx \le Cm\,,
$$

and so

$$\mathrm{Tr}\big[\sqrt{-\Delta+m^2}-m-\big(\gamma|\hat{x}|^{-1}+C\gamma m\big)\chi_{\{|x|<m^{-1}\}}\big]_-\geq -C(\gamma^{5/2}+\gamma^4)m\,. \tag{163}$$

Combining (162) and (163), and using $\gamma=2M\nu\alpha$, $\nu\alpha\leq 2/\pi$, we get that

$$\begin{aligned}&\mathrm{Tr}\big[\sqrt{-\alpha^{-2}\Delta+m^2\alpha^{-4}}-m\alpha^{-2}-\big(2\nu M|\hat{x}|^{-1}+C\nu Mm\alpha^{-1}\big)\chi_{\{|x|<\alpha m^{-1}\}}\big]_-\\ \geq\ & -C\alpha^{-2}(\gamma^{5/2}+\gamma^4)m\geq -C\nu^{5/2}\alpha^{1/2}m\,.\end{aligned} \tag{164}$$

Combining (160), (161), and (164), yields (32) for $\nu\alpha\leq 3/(16\pi M)$.

Assume now that $\nu\alpha\in[3/(16\pi M),2/\pi]$.

Let $\theta\in C_0^\infty(\mathbb{R}^3)$ satisfy $0\leq\theta(x)\leq 1$, $\theta(x)=1$ for $|x|\leq\alpha m^{-1}/4$, $\theta(x)=0$ for $|x|\geq\alpha m^{-1}/2$, $(1-\theta^2)^{1/2}\in C^1(\mathbb{R})$, and

$$\|\nabla\theta\|_\infty\leq C\alpha^{-1}m,\quad \|\nabla(1-\theta^2)^{1/2}\|_\infty\leq C\alpha^{-1}m\,.$$

Let $\theta_j(x)=\theta(x-R_j)$, $j=1,\ldots,M$, and $\theta_{M+1}(x)=(1-\sum_{j=1}^M\theta_j^2)^{1/2}$ (the latter is well-defined due to the assumption $\min_{k\neq\ell}|R_k-R_\ell|>2\alpha m^{-1}$). The relativistic IMS formula and the localisation estimate (26) used for Ω_j, $j=1,\ldots,M$, being the balls centered at R_j with radii $3\alpha m^{-1}/4$ and $\ell=\alpha m^{-1}/4$, and Ω_{M+1} being the (disjoint) union of the same balls and $\ell=\alpha m^{-1}/8$, gives the operator inequality

$$\begin{aligned}&\sqrt{-\alpha^{-2}\Delta+m^2\alpha^{-4}}-m\alpha^{-2}+W(\hat{x})\\ \geq\ &\theta_{M+1}\big(\sqrt{-\alpha^{-2}\Delta+m^2\alpha^{-4}}-m\alpha^{-2}-Cm\alpha^{-2}\sum_{j=1}^M\chi_{\Omega_j}+W(\hat{x})\big)\theta_{M+1}\\ +\ &\sum_{j=1}^M\theta_j\big(\sqrt{-\alpha^{-2}\Delta+m^2\alpha^{-4}}-m\alpha^{-2}-Cm\alpha^{-2}+W(\hat{x})\big)\theta_j-\sum_{j=1}^{M+1}Q_j\,,\end{aligned} \tag{165}$$

with

$$\mathrm{Tr}\big[Q_j\big]\leq C\,m\alpha^{-2}\,.$$

Here we have used that $\theta_i\chi_{\Omega_j}\theta_i=\delta_{ij}\,\theta_i{}^2$, $i,j\in\{1,\ldots,M\}$, $\theta_{M+1}\chi_{\Omega_{M+1}}\theta_{M+1}=0$, and $\theta_i\chi_{\Omega_{M+1}}\theta_i\leq\theta_i^2$, $i\neq M+1$.

Using the Daubechies inequality on the first term in (165) and the assumption on W in the second (noticing that $\theta_j(x)/d_{\mathbf{R}}(x)=\theta_j(x)/|x-R_j|$ due to the assumption $\min_{k\neq\ell}|R_k-R_\ell|>2\alpha m^{-1}$), we get from this that

$$\begin{aligned}&\mathrm{Tr}[\sqrt{-\alpha^{-2}\Delta+m^2\alpha^{-4}}-m\alpha^{-2}+W(\hat{x})]_-\\ \geq\ & -Cm^{3/2}\int_{d_{\mathbf{R}}(x)>\alpha m^{-1}/4}|W(x)|^{5/2}\,dx-C\alpha^3\int_{d_{\mathbf{R}}(x)>\alpha m^{-1}/4}|W(x)|^4\,dx-C\,m\alpha^{-2}\\ &-C\sum_{j=1}^M\big(m^{3/2}(m\alpha^{-2})^{5/2}+\alpha^3(m\alpha^{-2})^4\big)\big|\{x\,|\,\tfrac14\alpha m^{-1}<|x-R_j|<\tfrac34\alpha m^{-1}\}\big|\\ &+\sum_{j=1}^M\mathrm{Tr}\big[\theta_j\big(\sqrt{-\alpha^{-2}\Delta+m^2\alpha^{-4}}-m\alpha^{-2}-Cm\alpha^{-2}-\frac{\nu}{|\hat{x}-R_j|}-C\nu m\alpha^{-1}\big)\theta_j\big]_-\,.\end{aligned} \tag{166}$$

By the translation invariance of $-\Delta$, the last term equals

$$M\,\mathrm{Tr}\big[\theta\big(\sqrt{-\alpha^{-2}\Delta+m^2\alpha^{-4}}-Cm\alpha^{-2}-C\nu m\alpha^{-1}-\nu|\hat{x}|^{-1}\big)\theta\big]_-\,,$$

and using the Lieb-Yau inequality (and the properties of θ and that $\nu\alpha \leq 2/\pi$),

$$\begin{aligned} &\mathrm{Tr}\big[\theta\big(\sqrt{-\alpha^{-2}\Delta + m^2\alpha^{-4}} - Cm\alpha^{-2} - C\nu m\alpha^{-1} - \nu|\hat{x}|^{-1}\big)\theta\big]_- \\ &\quad\geq \ \alpha^{-1}\,\mathrm{Tr}\big[\theta\big(\sqrt{-\Delta} - \frac{2}{\pi}|\hat{x}|^{-1} - Cm\alpha^{-1}\big)\theta\big]_- \geq \ -Cm\alpha^{-2}\,. \end{aligned} \tag{167}$$

Further, by the assumption on W, and the assumption $\min_{k\neq\ell}|R_k - R_\ell| > 2\alpha m^{-1}$,

$$\begin{aligned} &m^{3/2}\int_{\alpha m^{-1}/4<d_{\mathbf{R}}(x)<\alpha m^{-1}} |W(x)|^{5/2}\,dx \\ &\quad\leq \sum_{j=1}^{M} C\nu^{5/2}m^{3/2}\int_{\alpha m^{-1}/4<|x-R_j|<\alpha m^{-1}} \big(|x-R_j|^{-1} + \alpha^{-1}m\big)^{5/2}\,dx \leq C\nu^{5/2}\alpha^{1/2}m\,, \end{aligned}$$

and, since $\nu\alpha \leq 2/\pi$,

$$\begin{aligned} &\alpha^{3}\int_{\alpha m^{-1}/4<d_{\mathbf{R}}(x)<\alpha m^{-1}} |W(x)|^{4}\,dx \\ &\quad\leq \sum_{j=1}^{M} C\nu^{4}\alpha^{3}\int_{\alpha m^{-1}/4<|x-R_j|<\alpha m^{-1}} \big(|x-R_j|^{-1} + \alpha^{-1}m\big)^{4}\,dx \leq C\nu^4\alpha^2 m \leq C\nu^{5/2}\alpha^{1/2}m\,. \end{aligned}$$

It follows from this, (167), and (166) that

$$\begin{aligned} &\mathrm{Tr}[\sqrt{-\alpha^{-2}\Delta + m^2\alpha^{-4}} - m\alpha^{-2} + W(\hat{x})]_- \\ &\quad\geq \ -Cm\alpha^{-2} - C\nu^{5/2}\alpha^{1/2}m - Cm^{3/2}\int_{d_{\mathbf{R}}(x)>\alpha m^{-1}} |W(x)|^{5/2}\,dx - C\alpha^3\int_{d_{\mathbf{R}}(x)>\alpha m^{-1}} |W(x)|^4\,dx\,. \end{aligned}$$

Since $m\alpha^{-2} \leq C\nu^{5/2}\alpha^{1/2}m$ when $\nu\alpha \in [3/(16\pi M), 2/\pi]$ this proves (32) in this case. This finishes the proof of Theorem 16. $\square$

Proof of Theorem 17 (**Correlation inequality**). The proof essentially uses superharmonicity and positive definiteness of $|x|^{-1}$ (see [19]). By superharmonicity and the spherical properties of Φ_s,

$$|x-y|^{-1} \geq \int \Phi_s(z-x)\,|z-z'|^{-1}\,\Phi_s(z'-y)\,dzdz'\,.$$

Also note that for the Coulomb energy, $D(\Phi_s,\Phi_s) = s^{-1}D(\Phi,\Phi) = Cs^{-1}$. Therefore, we immediately get that

$$\begin{aligned}
&\sum_{1\le i<j\le N} |x_i - x_j|^{-1} \\
&\ge \sum_{1\le i<j\le N} \int \Phi_s(z-x_i)\,|z-z'|^{-1}\,\Phi_s(z'-x_j)\,dzdz' \\
&= \tfrac12 \int \Big(\sum_{1\le j\le N} \Phi_s(z-x_j)\Big)\,|z-z'|^{-1}\,\Big(\sum_{1\le j\le N}\Phi_s(z'-x_j)\Big)\,dzdz' \\
&\quad - \tfrac{N}{2}\int \Phi_s(z)|z-z'|^{-1}\,\Phi_s(z')\,dzdz' \\
&= \tfrac12 \int \Big(\sum_{1\le j\le N} \Phi_s(z-x_j)-\rho(z)\Big)\,|z-z'|^{-1}\,\Big(\sum_{1\le j\le N}\Phi_s(z'-x_j)-\rho(z')\Big)\,dzdz' \\
&\quad + \int \rho(z)\,|z-z'|^{-1}\sum_{1\le j\le N}\Phi_s(z'-x_j)\,dzdz' \\
&\quad - \tfrac12\int \rho(z)\,|z-z'|^{-1}\,\rho(z')\,dzdz' - ND(\Phi_s,\Phi_s) \\
&\ge \sum_{1\le j\le N} \big(\rho * |x|^{-1} * \Phi_s\big)(x_j) - D(\rho) - CNs^{-1}\,.
\end{aligned}$$

In the last inequality we have used the positive definiteness of $|x|^{-1}$ and dropped the first term. This proves inequality (33). □

Proof of Corollary 21 (**Estimate on** $\rho^{\mathrm{TF}} * |x|^{-1} * (\delta_0 - \Phi_t)$). Let, with $d_{\mathbf{r}}$ as in (4),

$$g_{\mathbf{r}}(x) = \min\{d_{\mathbf{r}}(x)^{-1/2}, d_{\mathbf{r}}(x)^{-2}\}\,. \tag{168}$$

We claim that for some constant $C>0$,

$$\big|\nabla\rho^{\mathrm{TF}} * |x|^{-1}\big| \le C g_{\mathbf{r}}(x)\,. \tag{169}$$

To prove this we distinguish two regions.

First, let $d_{\mathbf{r}}(x)\ge 1$. Then $g_{\mathbf{r}}(x) = d_{\mathbf{r}}(x)^{-2}$. Using that $|\nabla V^{\mathrm{TF}}|(x) \le C g_{\mathbf{r}}(x)^2 d_{\mathbf{r}}(x)^{-1} = d_{\mathbf{r}}(x)^{-5}$ we obtain

$$\begin{aligned}
\big|\nabla\rho^{\mathrm{TF}} * |x|^{-1}\big| &= \Big|\nabla\Big(\sum_{j=1}^M z_j|x-r_j|^{-1} - V^{\mathrm{TF}}(x)\Big)\Big| \\
&\le \sum_{j=1}^M z_j|x-r_j|^{-2} + d_{\mathbf{r}}(x)^{-5} \le M\max_j\{z_j\}\big(\min_j|x-r_j|\big)^{-2} + d_{\mathbf{r}}(x)^{-5} \\
&= Cd_{\mathbf{r}}(x)^{-2} + d_{\mathbf{r}}(x)^{-5} \le Cg_{\mathbf{r}}(x)\,.
\end{aligned}$$

If on the other hand $d_{\mathbf{r}}(x)<1$, then, by using (36) and (41),

$$\begin{aligned}
\big|\nabla\rho^{\mathrm{TF}} * |x|^{-1}\big| &\le \int \big|\nabla\rho^{\mathrm{TF}}(y)\big|\,|x-y|^{-1}\,dy \le C\int g_{\mathbf{r}}(y)^3 d_{\mathbf{r}}(y)^{-1}\,|x-y|^{-1}\,dy \\
&= C\sum_{j=1}^M \int_{d_{\mathbf{r}}(y)=|y-r_j|} g_{\mathbf{r}}(y)^3 d_{\mathbf{r}}(y)^{-1}\,|x-y|^{-1}\,dy\,.
\end{aligned}$$

Since $g_{\mathbf{r}}(y) \le d_{\mathbf{r}}(y)^{-1/2} = |y-r_j|^{-1/2}$ when $d_{\mathbf{r}}(y) = |y-r_j|$ this implies that

$$\begin{aligned}
\left|\nabla\rho^{\mathrm{TF}} * |x|^{-1}\right| &\le C\sum_{j=1}^{M}\int |y-r_j|^{-5/2}\,|x-y|^{-1}\,dy \\
&= C\sum_{j=1}^{M}|x-r_j|^{-1/2} \le CMd_{\mathbf{r}}(x)^{-1/2} = Cg_{\mathbf{r}}(x)\,.
\end{aligned}$$

This finishes the proof of (169).

Let us now proceed to prove inequality (43). That the difference is positive is again just superharmonicity of $|x|^{-1}$. It is easy to see that

$$|d_{\mathbf{r}}(x) - d_{\mathbf{r}}(y)| \le |x-y|\,. \tag{170}$$

In the case when $d_{\mathbf{r}}(x) \ge 2t$ we can conclude that

$$\begin{aligned}
\rho^{\mathrm{TF}} * |x|^{-1} - \rho^{\mathrm{TF}} * |x|^{-1} * \Phi_t &\le \sup_{|z-x|\le t}\left\{\left|\nabla\rho^{\mathrm{TF}} * |z|^{-1}\right|\right\}\int |x-y|\,\Phi_t(x-y)\,dy \\
&\le Ct\sup_{|z-x|\le t} g_{\mathbf{r}}(z) \le Ctg_{\mathbf{r}}(x)\,.
\end{aligned}$$

In the last step we have used that if $d_{\mathbf{r}}(x) \ge 2t$ and $|z-x| \le t$ (this condition stems from the support of Φ_t), then inequality (170) guarantees that $\frac{1}{2}d_{\mathbf{r}}(x) \le d_{\mathbf{r}}(z) \le \frac{3}{2}d_{\mathbf{r}}(x)$. This in turn implies $(\frac{3}{2})^{-2}g_{\mathbf{r}}(x) \le g_{\mathbf{r}}(z) \le (\frac{1}{2})^{-1/2}g_{\mathbf{r}}(x)$.

If, on the other hand, $d_{\mathbf{r}}(x) \le 2t$, then we claim that

$$\left|\rho^{\mathrm{TF}} * |x|^{-1} - \rho^{\mathrm{TF}} * |y|^{-1}\right| \le C|x-y|^{1/2}\,. \tag{171}$$

This can be seen as follows.

$$\begin{aligned}
\left|\rho^{\mathrm{TF}} * |x|^{-1} - \rho^{\mathrm{TF}} * |y|^{-1}\right| &= \left|\int_0^1 \frac{d}{d\theta}\Big(\rho^{\mathrm{TF}} * |\theta x + (1-\theta)y|^{-1}\Big)\,d\theta\right| \\
&= \left|\int_0^1 \nabla\Big(\rho^{\mathrm{TF}} * |\theta x + (1-\theta)y|^{-1}\Big)\cdot(x-y)\,d\theta\right| \\
&\le C\int_0^1 g_{\mathbf{r}}(\theta x + (1-\theta)y)\,|x-y|\,d\theta \\
&\le C|x-y|\sum_{j=1}^{M}\int_0^1 |\theta x + (1-\theta)y - r_j|^{-1/2}\,d\theta \\
&= C|x-y|^{1/2}\sum_{j=1}^{M}\int_0^1 \left|\frac{\theta(x-y)}{|x-y|} + \frac{y-r_j}{|x-y|}\right|^{-1/2}\,d\theta\,.
\end{aligned}$$

Let $n = (x-y)/|x-y|$, $b = (y-r_j)/|x-y|$, and $c = n\cdot b$. Then $|\theta n + b|^2 \ge |\theta + n\cdot b|^2 = (\theta+c)^2$. Therefore

$$\left|\rho^{\mathrm{TF}} * |x|^{-1} - \rho^{\mathrm{TF}} * |y|^{-1}\right| \le C|x-y|^{1/2}\sum_{j=1}^{M}\int_0^1 |\theta+c|^{-1/2}\,d\theta\,.$$

The integral $\int_0^1 |\theta+c|^{-1/2}\,d\theta$ is bounded uniformly for $c \in \mathbb{R}$. This proves (171).

This allows us finally to show that for $d_{\mathbf{r}}(x) \leq 2t$,

$$\begin{aligned}
\rho^{\mathrm{TF}} * |x|^{-1} - \rho^{\mathrm{TF}} * |x|^{-1} * \Phi_t &= \int \big(\rho^{\mathrm{TF}} * |x|^{-1} - \rho^{\mathrm{TF}} * |y|^{-1}\big)\Phi_t(x-y)\,dy \\
&\leq C \int |x-y|^{1/2}\,\Phi_t(x-y)\,dy = Ct^{1/2}\,.
\end{aligned}$$

This finishes the proof of the corollary. □

Appendix B. Estimates of semi-classical integrals

In this appendix we give the remaining arguments on the analysis of the integrals in the semi-classical proofs of Lemma 33 and Lemma 34.

Proof of Lemma 33 (**Lower bound on** $\mathrm{Tr}[\phi H_\beta \phi]_-$): **Estimate of integral** (131). It remains to estimate the integral in (131). Note that by Taylor's formula for $\widetilde{\sigma}$ we have

$$\begin{aligned}
H^{(\varepsilon)}_{u,q}(v,p) \;\geq\; &\widetilde{\sigma}(v,p) + \widetilde{\xi}_{v,p}(u-v,q-p) - C|u-v|(b^{-1}+|u-v|^2) \\
&- C|q-p|(b^{-1}+|q-p|^2)\,,
\end{aligned} \tag{172}$$

where

$$\widetilde{\xi}_{v,p}(u,q) = \tfrac{1}{4b}\Delta\widetilde{\sigma}(v,p) - (1-\varepsilon)\tfrac{1}{2}\sum_{i,j}\partial_i\partial_j T_\beta(p) q_i q_j - \tfrac{1}{2}\sum_{i,j}\partial_i\partial_j V(v) u_i u_j\,.$$

We have used that $|\Delta\widetilde{\sigma}(v,p) - \Delta\widetilde{\sigma}(u,q)| \leq C|u-v| + C|q-p|$, and similarly, when replacing $\partial_i\partial_j F(q)$ by $\partial_i\partial_j F(p)$, and $\partial_i\partial_j V(u)$ by $\partial_i\partial_j V(v)$. We get that:

$$H^{(\varepsilon)}_{u,q}(v,p) \leq 0 \quad\Rightarrow\quad |p| \leq C\big(1 + |u-v|^3 + |q-p|^3\big)\,. \tag{173}$$

(Note that this holds also for $\varepsilon = 0$, and uniformly in $\beta \in [0,1]$; to see the latter, use that $T_\beta(p) \geq T_1(p)$.) This implies that

$$\int_{H^{(\varepsilon)}_{u,q}(v,p)\leq 0} \big(|u-v|^m + |q-p|^m\big) G_b(u-v) G_b(q-p)\,dp\,du\,dq \leq Cb^{-m/2}\,, \tag{174}$$

and

$$\int_{H^{(\varepsilon)}_{u,q}(v,p)\leq 0} \big(|u-v|^m + |q-p|^m\big) G_b(u-v) G_b(q-p)\,dp\,dv\,dq \leq Cb^{-m/2}\,. \tag{175}$$

From this we obtain that

$$\int G_b(u-v) G_b(q-p)\Big[H^{(\varepsilon)}_{u,q}(v,p)\Big]_-\,dp\,dq\,dv \geq -C\,, \tag{176}$$

and hence from (131) that

$$\begin{aligned}
&\mathrm{Tr}[\phi H_\beta \phi]_- \\
&\geq \int_{u\in B_2} \phi(v + h^2 ab(u-v))^2 G_b(u-v) G_b(q-p)\,[H_{u,q}(v,p)]_-\,\frac{du\,dq}{(2\pi h)^n}\,dv\,dp \\
&\quad - Ch^{-n}(b^{-3/2} + h^2 b)\,.
\end{aligned}$$

Here we have used the fact that the u-integration is over a bounded region. From now on we may however ignore the restriction on the u-integration. We note that, by using (173) and (174), that ϕ has support in B_1, and that $b > 1$, we get that

$$\int_{H^{(\varepsilon)}_{u,q}(v,p)\le 0} \phi(v + h^2 ab(u - v))^2 \big(|u - v|(b^{-1} + |u - v|^2) + |q - p|(b^{-1} + |q - p|^2)\big) \times G_b(u - v)G_b(q - p)\, dudqdvdp \le Cb^{-3/2}\,.$$

Using this and (172) we find after the simple change of variables $u \to u + v$ and $q \to q + p$ that

$$\begin{aligned}
&\mathrm{Tr}[\phi H_\beta \phi]_- \\
&\quad \ge \int \phi(v + h^2 abu)^2 G_b(u)G_b(q) \\
&\qquad \times \big[\widetilde{\sigma}(v, p) + \widetilde{\xi}_{v,p}(u, q) - C|u|(b^{-1} + |u|^2) - C|q|(b^{-1} + |q|^2)\big]_- \frac{dudq}{(2\pi h)^n} dvdp \\
&\qquad - Ch^{-n}(b^{-3/2} + h^2 b) \\
&\quad \ge \int \phi(v + h^2 abu)^2 G_b(u)G_b(q)\big[\widetilde{\sigma}(v, p) + \widetilde{\xi}_{v,p}(u, q)\big]_- \frac{dudq}{(2\pi h)^n} dvdp \\
&\qquad - Ch^{-n}(b^{-3/2} + h^2 b)\,.
\end{aligned} \tag{177}$$

At this point we divide the (v, p)-integration into three regions given in terms of a parameter $\Lambda > 0$ by

$$\Omega_- = \{(v, p) \mid \widetilde{\sigma}(v, p) \le -\Lambda\}\,,\ \Omega_+ = \{(v, p) \mid \widetilde{\sigma}(v, p) \ge \Lambda\}\,,\ \Omega_0 = \{(v, p) \mid |\widetilde{\sigma}(v, p)| < \Lambda\}\,.$$

The parameter Λ will be chosen such that $1 \ge \Lambda \ge Cb^{-1}$ for some sufficiently large constant C. This is possible if τ is small enough and hence b large enough. Then, since all the second derivatives of $\widetilde{\sigma}$ are bounded we may assume that $\frac{1}{4b}|\Delta\widetilde{\sigma}(v, p)| < \Lambda/2$ for all (v, p), uniformly in β.

We first consider Ω_+. We see from (177) that we only need to integrate over the set $\{(u, q) \,|\, C(|u|^2 + |q|^2) \ge \Lambda\}$. Also notice that $\widetilde{\sigma}(v, p) \ge \frac{1}{2}|p| - C$ (since $T_\beta(p) \ge T_1(p)$) shows that we only need to integrate over the set $\{p \mid |p| \le C(1 + |q|^2 + |u|^2)\}$. Therefore,

$$\int_{(v,p)\in\Omega_+} \phi(v + h^2 abu)^2 G_b(u)G_b(q)\big[\widetilde{\sigma}(v, p) + \widetilde{\xi}_{v,p}(u, q)\big]_-\, dudqdvdp \ge\ - C\mathrm{e}^{-Cb\Lambda}\,.$$

A similar argument shows that on Ω_- we can ignore the negative part $[\ \ ]_-$ paying the same price $-Ch^{-n}\mathrm{e}^{-Cb\Lambda}$.

For $(v, p) \in \Omega_-$ we estimate the integral

$$\int \phi(v + h^2 abu)^2 G_b(u)G_b(q)\big[\widetilde{\sigma}(v, p) + \widetilde{\xi}_{v,p}(u, q)\big]\, dudq \ge (\phi(v)^2 + Ch^2 b)\widetilde{\sigma}(v, p) - Ch^2 b\,.$$

Here we have expanded ϕ^2 to second order at the point v and used the crucial fact that

$$\int \widetilde{\xi}_{v,p}(u, q)G_b(u)G_b(q)\, dudq = 0\,. \tag{178}$$

For $(v,p)\in\Omega_-$ we have, of course, $\widetilde{\sigma}(v,p)=\widetilde{\sigma}(v,p)_-$. Since the volume of Ω_- is bounded by a constant we get for the integration over $\Omega_-\cup\Omega_+$,

$$\int\limits_{(v,p)\in\Omega_-\cup\Omega_+}\phi(v+h^2abu)^2G_b(u)G_b(q)\big[\widetilde{\sigma}(v,p)+\widetilde{\xi}_{v,p}(u,q)\big]_-\,dudqdvdp$$
$$\geq\int\limits_{(v,p)\in\Omega_-\cup\Omega_+}\phi(v)^2\widetilde{\sigma}(v,p)_-\,dvdp-C(h^2b+\mathrm{e}^{-Cb\Lambda})\,. \tag{179}$$

Finally, let $(v,p)\in\Omega_0$. Observe that, with $\vartheta(t)=(2t+\beta t^2)^{n/2}$,

$$\int\limits_{(v,p)\in\Omega_0}dp=c_n\big(\vartheta(-[\Lambda-V(v)]_-)-\vartheta(-[\Lambda+V(v)]_-)\big)\leq C\Lambda\,, \tag{180}$$

by the mean value theorem (uniformly in v). Now,

$$\begin{aligned}&\phi(v+h^2abu)^2\,G_b(u)G_b(q)\big[\widetilde{\sigma}(v,p)+\widetilde{\xi}_{v,p}(u,q)\big]_-\\&\quad\geq\;\phi(v+h^2abu)^2\,G_b(u)G_b(q)\big[\widetilde{\sigma}(v,p)\big]_-\\&\qquad-C\phi(v+h^2abu)^2\,G_b(u)G_b(q)(b^{-1}+|u|^2+|q|^2)\,,\end{aligned}$$

and, using the observation above and making the change of variables $v\to v-h^2abu$ in the v-integral,

$$\int\limits_{(v,p)\in\Omega_0}\phi(v+h^2abu)^2\,G_b(u)G_b(q)(b^{-1}+|u|^2+|q|^2)\,dvdpdudq\leq C\Lambda b^{-1}\,.$$

Expanding ϕ^2 to first order at v we have that

$$\begin{aligned}&\int\limits_{(v,p)\in\Omega_0}\phi(v+h^2abu)^2\,G_b(u)G_b(q)\widetilde{\sigma}(v,p)_-\,dvdpdudq\\&\quad\geq\int\limits_{(v,p)\in\Omega_0}\phi(v)^2\widetilde{\sigma}(v,p)_-\,dvdp\;+\;Ch^2ab\int\limits_{(v,p)\in\Omega_0,v\in\operatorname{supp}V}|u|\,G_b(u)G_b(q)\widetilde{\sigma}(v,p)_-\,dudqdvdp\\&\quad\geq\int\limits_{(v,p)\in\Omega_0}\phi(v)^2\widetilde{\sigma}(v,p)_-\,dvdp-Chb^{1/2}\Lambda^2\,.\end{aligned}$$

As a consequence,

$$\int\limits_{(v,p)\in\Omega_0}\phi(v+h^2abu)^2\,G_b(u)G_b(q)\big[\widetilde{\sigma}(v,p)+\widetilde{\xi}_{v,p}(u,q)\big]_-\,dudqdvdp$$
$$\geq\int\limits_{(v,p)\in\Omega_0}\phi(v)^2\widetilde{\sigma}(v,p)_-\,dvdp-C\Lambda(\Lambda hb^{1/2}+b^{-1})\,. \tag{181}$$

Since

$$\begin{aligned}
&\int \phi(v)^2 \widetilde{\sigma}(v,p)_-\, dvdp \\
&\quad= (1-\varepsilon)^{-n} \int \phi(v)^2 \big[\sqrt{\beta^{-1}p^2 + (1-\varepsilon)^2\beta^{-2}} - (1-\varepsilon)\beta^{-1} + V(v)\big]_-\, dvdp \\
&\quad\geq (1-\varepsilon)^{-n} \int \phi(v)^2 \sigma_\beta(v,p)_-\, dvdp \\
&\quad\geq \int \phi(v)^2 \sigma_\beta(v,p)_-\, dvdp - C\varepsilon\,,
\end{aligned}$$

the lemma follows from (177), (179), and (181) if we choose $b = h^{-4/5}$. □

Proof of Lemma 34 (**Construction of a trial density**): **Estimates of integrals**. We give here the remaining arguments on the analysis of the integrals in the semi-classical proofs of Lemma 34.

The energy: proof of (132)**.** It remains to estimate the integral in (139).

Using (173), that $T_\beta(p) \leq \frac{1}{2}p^2$, and that $h_{u,q}(v,p) = 0$ unless $u \in B_2$, we get that

$$\int \chi[h_{u,q}(v,p)]\, G_b(u-v) G_b(q-p) \big(1 + T_\beta(p + h^2 ab(q-p))\big)\, dudqdvdp \leq C\,.$$

This implies that

$$\begin{aligned}
&\mathrm{Tr}[\gamma\phi H_\beta \phi] \\
&\quad\leq \int \chi[h_{u,q}(v,p)]\, G_b(u-v) G_b(q-p) \phi\big(v + h^2 ab(u-v)\big)^2 \\
&\qquad\qquad \times \sigma\big(v + h^2 ab(u-v), p + h^2 ab(q-p)\big) \frac{dudq}{(2\pi h)^n} dvdp + Ch^2 bh^{-n}\,.
\end{aligned}$$

From (137) we may now conclude that

$$\begin{aligned}
&\mathrm{Tr}[\gamma\phi H_\beta\phi] \\
&\quad\leq \int_{u\in B_2 - v} \chi\big[\sigma(v,p) + \xi_{v,p}(u,q) - C|u|(b^{-1} + |u|^2) - C|q|(b^{-1}+|q|^2)\big]\, G_b(u) G_b(q) \\
&\qquad\qquad \times \phi(v + h^2 abu)^2 \sigma(v + h^2 abu, p + h^2 abq) \frac{dudq}{(2\pi h)^n} dvdp \,+\, Ch^2 bh^{-n}\,. \qquad (182)
\end{aligned}$$

At this point we introduce the same partition of the (v,p)-integration into sets $\Omega_\pm, \Omega_0$ as in the proof of the lower bound above (with $\varepsilon = 0$) with the same $\Lambda = b^{-1/2} = h^{2/5}$.

Then for the integration over Ω_+ we have as above that $C(|u|^2 + |q|^2) > \Lambda$ and hence

$$\begin{aligned}
&\int_{\substack{(v,p)\in\Omega_+,\\ u\in B_2 - v}} \chi\big[\sigma(v,p) + \xi_{v,p}(u,q) - C|u|(b^{-1}+|u|^2) - C|q|(b^{-1}+|q|^2)\big] \\
&\quad\times \phi(v+h^2abu)^2 \sigma(v+h^2abu, p+h^2abq)\, G_b(u)G_b(q)\, dudqdvdp \leq C\,\mathrm{e}^{-cb\Lambda} \leq Ch^2 b\,,
\end{aligned}$$

where we have used (136) and that ϕ is supported in the ball B_1.

Similarly, if $(v,p) \in \Omega_-$ then for the (u,q)-integration we can safely assume that the argument of χ is negative to the effect of paying the same $\mathrm{e}^{-Cb\Lambda}$ price. Likewise we may ignore the restriction $u \in B_2 - v$, since $u \notin B_2 - v$ and $v + h^2 abu \in B_1$ implies $|u| >$

$(1-h^2ab)^{-1} > 1$. Expanding ϕ^2 and σ to second order at $(v,p)\in\Omega_-$ and using the fact that all their second order derivatives are bounded together with (130) we get that

$$\begin{aligned}
&\int \chi\big[\sigma(v,p)+\xi_{v,p}(u,q)-C|u|(b^{-1}+|u|^2)-C|q|(b^{-1}+|q|^2)\big]\\
&\qquad\qquad\qquad\times\phi(v+h^2abu)^2\sigma(v+h^2abu,p+h^2abq)\,G_b(u)G_b(q)\,dudq\\
\le\ &\int\Big[\big(\phi(v)^2+h^2ab\,u\cdot\nabla(\phi^2)(v)\big)\big(\sigma(v,p)+h^2ab\,(u,q)\cdot\nabla\sigma(v,p)\big)\Big]\,G_b(u)G_b(q)\,dudq\\
&+Ch^2b+C\,\mathrm{e}^{-Cb\Lambda}\\
\le\ &\phi(v)^2\sigma(v,p)_-+Ch^2b\,.
\end{aligned}$$

It is important here that σ and $\nabla\sigma$ are bounded uniformly in $\beta\le 1$ on Ω_-. This follows from (136) and $|\nabla\sigma_\beta(v,p)|\le C(1+|p|)$. Indeed, (136), in particular, implies that Ω_- is a bounded set (uniformly in β). The fact that the volume of Ω_- is bounded also gives that the contribution from Ω_- to the integral on the right side of (182) is bounded above by

$$(2\pi h)^{-n}\int_{\Omega_-}\phi(v)^2\sigma(v,p)_-dvdp+Ch^2bh^{-n}.$$

Finally, we consider $(v,p)\in\Omega_0$. If we expand ϕ^2 to first order at v and σ to second order at (v,p) and use that all second order derivatives of σ are bounded and that $\nabla\sigma(v,p)$ is bounded for $(v,p)\in\Omega_0$ we obtain that

$$\phi(v+h^2abu)^2\sigma(v+h^2abu,p+h^2abq)\le\phi(v)^2\sigma(v,p)+Ch^2ab(|u|+|q|)+Ch^4a^2b^2(|u|^2+|q|^2).$$

This together with the estimate $|\chi(x+y)x-\chi(x)x|\le|y|$ implies that

$$\begin{aligned}
&\int_{u\in B_2-v}\chi\big[\sigma(v,p)+\xi_{v,p}(u,q)-C|u|(b^{-1}+|u|^2)-C|q|(b^{-1}+|q|^2)\big]\\
&\qquad\qquad\qquad\times\phi(v+h^2abu)^2\sigma(v+h^2abu,p+h^2abq)\,G_b(u)G_b(q)\,dudq\\
\le\ &\int\chi[\sigma(v,p)+\xi_{v,p}(u,q)-C|u|(b^{-1}+|u|^2)-C|q|(b^{-1}+|q|^2)]\,G_b(u)G_b(q)\,dudq\\
&\qquad\qquad\times\phi(v)^2\sigma(v,p)+Ch^2b^{3/2}\\
\le\ &\phi(v)^2\sigma(v,p)_-+C(b^{-1}+h^2b^{3/2})\,.
\end{aligned}$$

We have here again used that the effect of removing the restriction $u\in B_2-v$ causes a smaller error than the last term above. Note that $u\in B_2-v$ and $v+h^2abu\in B_1$ imply $|u|\le 3(1-h^2ab)^{-1}\le 6$ and hence we only need to consider $|v|\le|v+u|+|u|<8$. If we use that (180) implies

$$\mathrm{Vol}(\Omega_0\cap\{v\mid |v|<8\}\times\mathbb{R}^n)\le C\Lambda$$

we see that the contribution from Ω_0 to the integral on the right side of (182) is bounded above by

$$(2\pi h)^{-n}\int_{\Omega_0}\phi(v)^2\sigma(v,p)_-\,dvdp+Ch^{-n}(b^{-1}+h^2b^{3/2})\Lambda\,.$$

This finishes the proof of the upper bound on the energy in (132) .

The density: proof of (133) **and** (134)**.** Here it remains to estimate the integral in (140). The strategy is to freeze the variable $|p|$ in $\xi_{v,p}$ so that the remaining dependence on $|p|$ is explicitly integrable. This is accomplished in the estimate (183) below. After the $|p|$-integration the proof is almost the same as in the non-relativistic case [36].

We write $p = |p|\omega$ and define

$$p_0 = (\beta|V(v)_-|^2 + 2|V(v)_-|)^{1/2}\omega = \eta(V(v))^{1/n}\omega\,.$$

We will then prove that if $u \in B_2 - v$ then

$$\chi[\sigma(v,p)+\xi_{v,p_0}(u,q)+R(u,q)] \leq \chi[h_{u+v,q+p}(v,p)] \leq \chi[\sigma(v,p)+\xi_{v,p_0}(u,q)-R(u,q)]\,, \tag{183}$$

where

$$R(u,q) = C(|u|(b^{-1}+|u|^2) + (|q|+\Lambda)(b^{-1}+|q|^2) + (b^{-1}+|u|^2+|q|^2)(|u|^2+|q|^2)\Lambda^{-1})\,.$$

We first prove (183) for $(v,p) \in \Omega_0$. In this case we have

$$\eta(V(v)+\Lambda)^{2/n} \leq p^2 \leq \eta(V(v)-\Lambda)^{2/n}\,,$$

from which it follows that $|p^2 - p_0^2| \leq C\Lambda$ with a constant independent of $\beta \in [0,1]$.

Let $G(t) = \sqrt{\beta^{-1}t + \beta^{-2}} - \beta^{-1}$, so that $T_\beta(p) = G(p^2)$ (we suppress that G depends on β). Note that then $\partial_i\partial_j T_\beta(p) = 4p_ip_jG''(p^2) + 2\delta_{ij}G'(p^2)$, and so, in particular, $\Delta T_\beta(p) = 4G''(p^2)p^2 + 2nG'(p^2)$. Therefore, using that $p_i = |p|\omega_i, p_{0,i} = |p_0|\omega_i$,

$$\begin{aligned}
&|\xi_{v,p}(u,q) - \xi_{v,p_0}(u,q)| \\
&\quad\leq \tfrac{1}{4b}\,|\Delta\sigma(v,p) - \Delta\sigma(v,p_0)| + \tfrac{1}{2}\sum_{i,j}\big|\partial_i\partial_j[T_\beta(p) - T_\beta(p_0)]\big|\,|q_iq_j| \\
&\quad\leq C(b^{-1}+|q|^2)\big(|G''(p^2)p^2 - G''(p_0^2)p_0^2| + |G'(p^2) - G'(p_0^2)|\big) \\
&\quad\leq C(b^{-1}+|q|^2)\,|p^2-p_0^2| \;\leq\; C\Lambda(b^{-1}+|q|^2)\,.
\end{aligned} \tag{184}$$

Here we have used the choice of p_0 and that $G'(t)$ and $tG''(t)$ have bounded derivatives uniformly in $\beta \in [0,1]$. If we combine (137) with (184) we obtain that

$$|h_{u+v,q+p}(v,p) - \sigma(v,p) - \xi_{v,p_0}(u,q)| \leq C|u|(b^{-1}+|u|^2) + |q|(b^{-1}+|q|^2) + C\Lambda(b^{-1}+|q|^2)\,,$$

which is, in fact, stronger than (183).

If $(v,p) \in \Omega_+$ we see that the left inequality in (183) is only violated if $\xi_{v,p_0}(u,q) \leq -\Lambda$ and the right inequality is only violated if $h_{u+v,q+p}(v,p) \leq 0$. Since $(v,p) \in \Omega_+$ we must in both cases have $C(|u|^2+|q|^2) > \Lambda$. We hence get (again using (137)) that

$$\begin{aligned}
&\big|h_{u+v,q+p}(v,p) - \sigma(v,p) - \xi_{v,p_0}(u,q)\big| \\
&\quad\leq \big|h_{u+v,q+p}(v,p) - \sigma(v,p) - \xi_{v,p}(u,q)\big| + \big|\xi_{v,p}(u,q)\big| + \big|\xi_{v,p_0}(u,q)\big| \\
&\quad\leq C|u|(b^{-1}+|u|^2) + C|q|(b^{-1}+|q|^2) + C(b^{-1}+|u|^2+|q|^2) \\
&\quad\leq C|u|(b^{-1}+|u|^2) + C|q|(b^{-1}+|q|^2) + C(b^{-1}+|u|^2+|q|^2)(|u|^2+|q|^2)\Lambda^{-1}\,,
\end{aligned}$$

which gives (183) in this case.

Finally, if $(v,p) \in \Omega_-$ then the left inequality in (183) is only violated if $h_{u+v,q+p}(v,p) \geq 0$ and the right inequality is only violated if $\xi_{v,p_0}(u,q) \geq \Lambda$. In both cases this implies that $C(|u|^2+|q|^2) > \Lambda$ and hence the same argument as for Ω_+ proves (183).

Using (183) we can estimate the density in (140) from above and below. We will discuss the lower bound on the density. The upper bound is similar. Performing the $|p|$-integral in

(140) we obtain

$$\begin{aligned}\rho_\gamma(x) &\geq \int\limits_{u\in B_2-v} \Xi(u,q,v,\omega)G_b(u)G_b(q)G_{(h^2b)^{-1}}(x-v-h^2abu)\,dvd\omega\,\frac{dudq}{(2\pi h)^n} \\ &= \int\limits_{(1-h^2ab)u\in B_2-v} \Xi(u,q,v-h^2abu,\omega)G_b(u)G_b(q)G_{(h^2b)^{-1}}(x-v)\,dvd\omega\,\frac{dudq}{(2\pi h)^n}\,,\end{aligned} \tag{185}$$

where

$$\Xi(u,q,v,\omega)=n^{-1}\eta\left(V(v)+\xi_{v,p_0}(u,q)+R(u,q)\right)\,.$$

We have that

$$\begin{aligned}&V(v-h^2abu)+\xi_{v-h^2abu,p_0}(u,q)+R(u,q)\\ &\quad\leq\ V(v)-h^2abu\nabla V(v)+\xi_{v,p_0}(u,q)+R(u,q)+Ch^4a^2b^2|u|^2+Ch^2ab|u|(b^{-1}+|u|^2)\\ &\quad\leq\ V(v)-h^2abu\nabla V(v)+\xi_{v,p_0}(u,q)+R(u,q)+Ch^4a^2b^2|u|^2\,.\end{aligned} \tag{186}$$

(In the last line we have used that $h^2ab\leq 1$ and the definition of $R(u,q)$.) We now use that

$$\big|\eta(s)-\eta(t)-\eta'(t)(s-t)\big|\leq\begin{cases} C|s-t|^{3/2}+C(|s|+|t|)|s-t|^2\,, & n=3\\ C(|s|^{\frac{n}{2}-2}+|t|^{\frac{n}{2}-2}+|s|^{n-2}+|t|^{n-2})|s-t|^2\,, & n\geq 4\end{cases}\,. \tag{187}$$

We continue with the case $n=3$ and leave $n\geq 4$ to the reader.

If we use the fact that $\eta'(V(v))$ is bounded independently of $\beta\in[0,1]$ we obtain from (186) and (187)

$$\begin{aligned}n\,\Xi(u,q,v-h^2abu,\omega)\ \geq\ &\eta(V(v))+\eta'(V(v))(\xi_{v,p_0}(u,q)-h^2abu\nabla V(v))\\ &-C\big(b^{-1}+|q|^2+|u|^2+h^2ab|u|+R(u,q)\big)^{3/2}\\ &-C\big(b^{-1}+|q|^2+|u|^2+h^2ab|u|+R(u,q)\big)^2\\ &-CR(u,q)-Ch^4a^2b^2|u|^2-Ch^2ab|u|\,.\end{aligned} \tag{188}$$

It is now crucial that (see (130) and (178))

$$\int\left(\xi_{v,p_0}(u,q)-h^2abu\nabla V(v)\right)G_b(u)G_b(q)\,dudq=0\,.$$

Since $v\in\mathrm{supp}(V)\subset B_{3/2}$ and $(1-h^2ab)u\notin B_2-v$ implies $|u|>1/2$ we find

$$\left|\ \int\limits_{(1-h^2ab)u\in B_2-v}\left(\xi_{v,p_0}(u,q)-h^2abu\nabla V(v)\right)G_b(u)G_b(q)\,dudq\right|\leq C\,\mathrm{e}^{-b/5}\leq Ch^{6/5}\,. \tag{189}$$

Combining this with (188) and inserting it into (185) we arrive at (recall that $\Lambda=b^{-1/2}$)

$$\begin{aligned}\rho_\gamma(x)\ \geq\ &(2\pi h)^{-3}\omega_3\int\eta\big[V(v)\big]G_{(h^2b)^{-1}}(x-v)\,dv\\ &-Ch^{-3}\big(h^{6/5}+b^{-3/2}+(h^2ab)^{3/2}b^{-3/4}\big)\,.\end{aligned} \tag{190}$$

Here we have removed the constraint $(1-h^2ab)u\in B_2-v$ by the same argument as above.

We shift the v-coordinate by x, and then expand $\eta\big[V(x+v)\big]$ in the integral at x by expanding V to second order at x and using (187). Then

$$\eta\big[V(x+v)\big]\geq\eta\big[V(x)\big]+\eta'\big[V(x)\big]\nabla V(x)\cdot v-C(|v|^{3/2}+|v|^3)\,.$$

Then we obtain from (190) (using (130)) that

$$\rho_\gamma(x) - (2\pi h)^{-3}\omega_3\,\eta\big[V(x)\big] \geq -Ch^{-3}\big(h^{6/5} + (h^2b)^{3/4}\big) \geq\, -Ch^{-3+9/10}\,.$$

This finishes the proof of (133).

Lastly, we prove (134). By integrating (190) we see that

$$\begin{aligned}
&\int \phi(x)^2 \rho_\gamma(x)\,dx \\
&\geq\ (2\pi h)^{-3}\omega_3 \int \phi(x)^2\, G_{(h^2b)^{-1}}(x-v)\,\eta\big[V(v)\big]\,dxdv - Ch^{-3+6/5} \\
&\geq\ (2\pi h)^{-3}\omega_3 \int \phi(v)^2\,\eta\big[V(v)\big]\,dv - Ch^{-3+6/5}\,.
\end{aligned}$$

In the last step we have expanded ϕ^2 to second order at v to obtain that (see also (130))

$$\int \phi(x)^2 G_{(h^2b)^{-1}}(x-v)\,dx \leq \phi(v)^2 + Ch^{6/5}\,.$$

This finishes the proof of (134) and therefore of Lemma 34. □

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