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To the memory of Michael Solomyak

ASYMPTOTICS OF THE GROUND STATE ENERGY IN THE RELATIVISTIC SETTINGS

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The paper is aimed at deriving sharp asymptotics of the ground state energy for the heavy atoms and molecules in the relativistic settings, and, in particular, calculating the relativistic Scott correction term and also Dirac, Schwinger, and relativistic correction terms. Also it is proved that the Thomas–Fermi density approximates the actual density of the ground state, which opens the way to estimate the excessive negative and positive charges and the ionization energy.

§1. Introduction

In this paper, our goal is to derive sharp asymptotics of the ground state energy for heavy atoms and molecules in the relativistic settings, and, in particular, to derive the relativistic Scott correction term and also the Dirac, Schwinger and relativistic correction terms. For the first time, the relativistic Scott correction term was derived in [13], which both inspired our paper and provided necessary functional analytic tools; our improvement is achieved due to more refined microlocal semiclassical techniques.

Also we will prove that the Thomas–Fermi density approximates the actual density of the ground state, which opens the way to estimate the excessive negative and positive charges and the ionization energy.

In the next paper [10] we will introduce a self-generated magnetic field and improve the results of [4].

Key words: relativistic Schrödinger operator, heavy atoms and molecules, Thomas–Fermi theory, Scott correction term, microlocal analysis, sharp spectral asymptotics.

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The multielectron Hamiltonian is given by

$$\mathsf{H} = \mathsf{H}_N := \sum_{1\leqslant j\leqslant N} H_{V,x_j} + \sum_{1\leqslant j<k\leqslant N} \frac{\mathsf{e}^2}{|x_j - x_k|} \tag{1.1}$$

on

$$\mathfrak{H} = \bigwedge_{1\leqslant n\leqslant N} \mathscr{H}, \qquad \mathscr{H} = \mathscr{L}^2(\mathbb{R}^3, \mathbb{C}^q) \simeq \mathscr{L}^2(\mathbb{R}^3 \times \{1, \dots, q\}, \mathbb{C}) \tag{1.2}$$

with

$$H_V = T - \mathsf{e}V(x), \tag{1.3}$$

describing N same type particles in the external field with the scalar potential $-V$ and repulsing one another in accordance with the Coulomb law; e is the charge of the electron, T is the *kinetic energy operator*.

In the nonrelativistic framework this operator is defined as

$$T = \frac{1}{2\mu}(-i\hbar\nabla)^2. \tag{1.4}$$

In the relativistic framework this operator is defined as

$$T = \Bigl(c^2(-i\hbar\nabla)^2 + \mu^2c^4\Bigr)^{\frac{1}{2}} - \mu^2c^4. \tag{1.5}$$

Here

$$V(x) = \sum_{1\leqslant m\leqslant M} \frac{Z_m\mathsf{e}}{|x - \mathsf{y}_m|} \tag{1.6}$$

and

$$d = \min_{1\leqslant m<m'\leqslant M} |\mathsf{y}_m - \mathsf{y}_{m'}| > 0, \tag{1.7}$$

where $Z_m\mathsf{e} > 0$ and y_m are the charges and locations of the nuclei.

It is well known that the nonrelativistic operator is always semibounded from below. On the other hand, it is also well known [8, 12] that the following is true.

Remark 1. A one particle relativistic operator is semibounded from below if and only if

$$Z_m\beta \leqslant \frac{2}{\pi} \quad \text{for all} \quad m = 1, \dots, M; \qquad \beta =: \frac{\mathsf{e}^2}{\hbar c}. \tag{1.8}$$

We will assume (1.8), sometimes replacing it by a strict inequality:

$$Z_m\beta \leqslant \frac{2}{\pi} - \epsilon \quad \text{for all} \quad m = 1, \dots, M; \qquad \beta =: \frac{\mathsf{e}^2}{\hbar c}. \tag{1.9}$$

We also assume that $d \geqslant CZ^{-1}$. Then we are interested in $\mathsf{E} := \inf \operatorname{Spec}(\mathsf{H})$.

Remark 2. (1) In the nonrelativistic theory, by scaling with respect to the spatial and energy variables we can make $\hbar = \mathsf{e} = \mu = 1$, while the Z_m are preserved.

(2) In the relativistic theory, by scaling with respect to the spatial and energy variables we can make $\hbar = \mathsf{e} = \mu = 1$, while β and the Z_m are preserved.

From now on we assume that such rescaling was already made and we are free to use the letters $\hbar$, μ, and c for other notations.

§2. Functional analytic arguments

2.1. Estimate from below. In contrast to [13], we start with a more traditional approach. We estimate

$$\sum_{1\leqslant j<k\leqslant N} \langle |x_j - x_k|^{-1}\Psi, \Psi\rangle$$

from below, using Lieb's electrostatic inequality, by

$$\frac{1}{2}\mathsf{D}(\rho_\Psi, \Psi) - C\int \rho_\Psi^{4/3}\, dx,$$

where $\langle\,\cdot\,,\,\cdot\,\rangle$ means the inner product in $\mathfrak{H}$, $\rho_\Psi(x)$ is a one particle density,

$$\mathsf{D}(\rho, \rho') = \iint |x-y|^{-1}\rho(x)\rho'(y)\, dxdy,$$

and we use the notation of Chapter 25 of [9].

Then the standard lower estimate [9, (25.2.2)] holds true:

$$\begin{aligned}\langle \mathsf{H}_N\Psi, \Psi\rangle &\geqslant \sum_{1\leqslant j\leqslant N} \langle H_{V,x_j}\Psi, \Psi\rangle + \frac{1}{2}\mathsf{D}\big(\rho_\Psi, \rho_\Psi\big) - C\int \rho_\Psi^{\frac{4}{3}}(x)\, dx\\ &= \sum_{1\leqslant j\leqslant N} \langle H_{W,x_j}\Psi, \Psi\rangle + \frac{1}{2}\mathsf{D}\big(\rho_\Psi - \rho, \rho_\Psi - \rho\big)\\ &\qquad\qquad - \frac{1}{2}\mathsf{D}\big(\rho, \rho\big) - C\int \rho_\Psi^{\frac{4}{3}}(x)\, dx,\end{aligned} \tag{2.1}$$

where H_W is the one-particle Schrödinger operator (respectively, nonrelativistic or relativistic) with the potential

$$W = V - |x|^{-1} * \rho, \tag{2.2}$$

and ρ is an arbitrarily chosen real-valued nonnegative function. Then again we get

$$\mathsf{E}_N \geqslant \operatorname{Tr}(H^-_{W+\lambda}) + \lambda N + \frac{1}{2}\mathsf{D}\big(\rho_\Psi - \rho, \rho_\Psi - \rho\big) - \frac{1}{2}\mathsf{D}\big(\rho, \rho\big) - C\int \rho_\Psi^{\frac{4}{3}}(x)\, dx \tag{2.3}$$

with λ arbitrary.

Remark 3. As usual, we will need to improve these estimates to recover a remainder estimate better than $O(Z^{\frac{5}{3}})$.

Now we need to prove the estimate

$$\int \rho_\Psi^{\frac{4}{3}}(x)\, dx \leqslant CZ^{\frac{5}{3}} \tag{2.4}$$

for the ground state energy. This follows from the inequality

$$\int \rho_\Psi^{\frac{5}{3}}(x)\, dx \leqslant CZ^{\frac{7}{3}}, \tag{2.5}$$

the identity $\int \rho_\Psi\, dx = N$, and the assumption $N \lesssim Z$. To prove (2.5), we apply the classical arguments of Lieb–Thirring, but replacing the Lieb–Thirring inequality by some relativistic inequalities (see Appendix 5). Namely, let $\mathsf{b} =: T - KU$ with

$$U = \rho_\Psi^{\frac{2}{3}}\varphi_< + \beta^{-1}\rho_\Psi^{\frac{1}{3}}\varphi_>,$$

where $\varphi_\gtrless$ is the characteristic function of $\{x\colon \rho_\Psi \gtrless \beta^{-3}\}$.

Consider the multiparticle operator $B = \sum \mathsf{b}_{x_j}$ and its lowest eigenvalue E_0. Obviously,

$$E_0 \leqslant \langle B\Psi, \Psi\rangle = \sum_j \langle T_{x_j}\Psi, \Psi\rangle - K\int \Big(\rho_\Psi^{\frac{5}{3}}\varphi_< + \beta^{-1}\rho_\Psi^{\frac{4}{3}}\varphi_>\Big)\, dx. \tag{2.6}$$

On the other hand, E_0 does not exceed the sum of the negative eigenvalues of b, and the Daubechies inequality (5.1) shows that the absolute value of this sum does not exceed

$$C_0\int \max\big(U^{\frac{5}{2}}, \beta^3 U^4\big)\, dx \leqslant C_0 K^{\frac{5}{2}}\int \Big(\rho_\Psi^{\frac{5}{3}}\varphi_< + \beta^{-1}\rho_\Psi^{\frac{4}{3}}\varphi_>\Big)\, dx. \tag{2.7}$$

Therefore, assuming that $E_0 \leqslant 0$, we conclude that

$$\sum_j \langle T_{x_j}\Psi, \Psi\rangle - K\int \min\Big(\rho_\Psi^{\frac{5}{3}}, \beta^{-1}\rho_\Psi^{\frac{4}{3}}\Big) + C_0 K^{\frac{5}{2}}\int \Big(\rho_\Psi^{\frac{5}{3}}\varphi_< + \beta^{-1}\rho_\Psi^{\frac{4}{3}}\varphi_>\Big)\, dx \geqslant 0,$$

and therefore, for a small positive constant K, we conclude that

$$\sum_j \langle T_{x_j}\Psi, \Psi\rangle \geqslant 2\epsilon_0 \int \Big(\rho_\Psi^{\frac{5}{3}}\varphi_< + \beta^{-1}\rho_\Psi^{\frac{4}{3}}\varphi_>\Big)\, dx. \tag{2.8}$$

Thus, we have proved that (2.8) is true for any $\Psi \in \mathfrak{H}$. Then

$$\begin{aligned}\sum_j \langle H_{x_j}\Psi,\Psi\rangle &= \sum_j \langle T_{x_j}\Psi,\Psi\rangle - \int V(x)\rho_\Psi(x)\,dx\\ &\geqslant \int \Bigl(2\epsilon_0\rho_\Psi^{\frac{5}{3}} - V(x)\rho_\Psi\Bigr)\varphi_<\,dx + \int\Bigl(2\epsilon_0\beta^{-1}\rho_\Psi^{\frac{4}{3}} - V(x)\rho_\Psi\Bigr)\varphi_>\,dx.\end{aligned}\tag{2.9}$$

We know that the last expression must be less than $-c_0 Z^{\frac{7}{3}}$ (this will follow, e.g., from the estimate from above). Observe that for $\ell(x)\geqslant aZ^{-\frac{1}{3}}$ we have $V(x) < a^{-1}Z^{\frac{4}{3}}$ and the integral over this zone of $-V\rho_\Psi$ is greater than $-C_0a^{-1}Z^{\frac{4}{3}}N$. Here and below $\ell(x) =: \ = \min_j |x-\mathsf{y}_j|$. We fix a, a sufficiently large constant.

Next,

$$\int\limits_{\{x\colon \ell(x)\leqslant aZ^{-1/3}\}} \Bigl(\epsilon_0\rho_\Psi^{\frac{5}{3}} - V(x)\rho_\Psi\Bigr)\varphi_<\,dx \geqslant -C \int\limits_{\{x\colon \ell(x)\leqslant aZ^{-1/3}\}} V^{\frac{5}{2}}\,dx \geqslant -C_1 Z^{\frac{7}{3}}$$

and $(\epsilon_0\beta^{-1}\rho_\Psi^{1/3} - V)\varphi_>$ is positive unless $\rho_\psi > \beta^{-3}$ and $V\geqslant \epsilon_1\beta^{-1}\rho_\Psi^{1/3}\geqslant \epsilon_1\beta^{-2}$ (and then $\ell(x)\leqslant C_0\beta$).

Therefore, we estimate $\int(\rho_\Psi^{5/3}\varphi_< + \beta^{-1}\rho_\Psi^{4/3}\varphi_<)\,dx$ from above by $CZ^{7/3}$ plus $\int_{\{x:\ell(x)\leqslant C\beta\}} V\rho_\Psi\,dx$, and to obtain (2.4), it suffices to estimate this term. Next, it suffices to replace V by V_m (because $V = V_m + O(\beta^2)$, provided the distances between the nuclei are at least $C\beta$). Also, we can replace V_m by $V_m + C\beta^{-2}$.

If $Z_m\beta \leqslant \frac{2}{\pi} - \epsilon$, then we can write $H = \eta(H - V^1) + (1-\eta)(H - V^0)$, where $(1-\eta)V^0$ coincides with V in the β-vicinity of y_m and equals 0 outside of the 2β-vicinity of it, and $V^1 = \eta^{-1}(V - (1-\eta)V^0)$, and apply all above arguments to the operator with $V = V^1$, while simply observing that $H - V^0$ is a positive operator for η sufficiently small. So we have proved the following claim.

Proposition 4. *Under the assumption* (1.9) *for the ground state, we have*

$$\int \min\Bigl(\beta^{-1}\rho_\Psi^{\frac{4}{3}}, \rho_\Psi^{\frac{5}{3}}\Bigr)\,dx \leqslant CZ^{\frac{7}{3}}\tag{2.10}$$

and (2.4) *is fulfilled.*

Then we immediately arrive to Statement 1 below, and Statement 2 follows from either [1, Theorem 1] or [7, Theorem 3].

Corollary 5. *Under the assumption* (1.9),

(1) *we have*

$$\mathsf{E}_N \geqslant \operatorname{Tr}(H^-_{W+\lambda}) - \frac{1}{2}\mathsf{D}(\rho,\rho) - CZ^{\frac{5}{3}} + \frac{1}{2}\mathsf{D}(\rho-\rho_\Psi,\, \rho-\rho_\Psi), \tag{2.11}$$

where ρ,λ *are arbitrary and* $W = V - |x|^{-1} * \rho$;

(2) *next,*

$$\begin{aligned}\mathsf{E}_N \geqslant \operatorname{Tr}(H^-_{W+\lambda}) &- \frac{1}{2}\mathsf{D}(\rho,\rho)\\ &- \frac{1}{2}\int |x-y|^{-1}\operatorname{tr}\bigl(e^\dagger_N(x,y)\, e_N(x,y)\bigr)\, dxdy\\ &- CZ^{\frac{5}{3}-\delta} + \frac{1}{2}\mathsf{D}(\rho-\rho_\Psi,\, \rho-\rho_\Psi),\end{aligned} \tag{2.12}$$

where $e_N(x,y)$ *is the Schwartz kernel of the projector to* N *lower eigestates of* H_W *and* tr *denotes the matrix trace.*

To cover[1] the critical case[2] we will use [13, (2.21)]:

$$\sum_{1\leqslant i<j\leqslant N} |x_i - x_j|^{-1} \geqslant \sum_{j=1}^N (\rho * |x|^{-1} * \Phi_s)(x_j) - \frac{1}{2}\mathsf{D}(\rho,\rho) - CN\varepsilon^{-1}, \tag{2.13}$$

where, again, $\rho \geqslant 0$ is arbitrary, and λ is arbitrary, $\Phi \geqslant 0$ is spherically symmetric with $\int \Phi\, dx = 1$, $\Phi_\varepsilon(x) = \varepsilon^{-3}\Phi(x/\varepsilon)$. Here the factor $\frac{1}{2}$ is due to the difference in notation, and also now we have

$$W =: W_\varepsilon = V - |x|^{-1} * \rho * \Phi_\varepsilon \tag{2.14}$$

instead of (2.2), and the term $-CNs^{-1}$ replaces the last term in (2.3).

Proposition 6. *Under the assumption* (1.8),

$$\mathsf{E}_N \geqslant \operatorname{Tr}(H^-_{W+\lambda}) + \lambda N - \frac{1}{2}\mathsf{D}(\rho,\rho) - CN\varepsilon^{-1}. \tag{2.15}$$

Remark 7. (1) Later we shall set $\varepsilon = Z^{-\frac{2}{3}}$. This would lead to an $O(Z^{\frac{5}{3}})$ remainder estimate.

(2) Proposition 6 is weaker than Corollary 5 in two ways: there is no improved version of corollary 5(ii) and also there is no "bonus term" $\frac{1}{2}\mathsf{D}(\rho-\rho_\Psi, \rho-\rho_\Psi)$ in the right-hand expression.

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[1] Unfortunately, only partially.

[2] I.e., with the nonstrict inequality (1.8) instead of (1.9).

2.2. Estimate from above. The estimate from above is straightforward: we simply take Ψ as a Slater determinant of N lower eigenfunctions of H_W. If there are only $N' < N$ negative eigenvalues, then we take only N' such eigenvalues, because $\mathsf{E}_N \leqslant \mathsf{E}_{N'}$. This yields the following.

Proposition 8.

$$\begin{aligned}\mathsf{E}_N \leqslant \operatorname{Tr}(H^-_{W+\lambda}) &- \frac{1}{2}\mathsf{D}(\rho,\rho) + |\lambda-\nu|\cdot|\mathsf{N}^-_{W+\nu} - N| \\ &+ \mathsf{D}(\operatorname{tr} e_N(x,x) - \rho,\, \operatorname{tr} e_N(x,x,\nu) - \rho) \\ &- \frac{1}{2}\int |x-y|^{-1}\operatorname{tr}\bigl(e^\dagger_N(x,y)e_N(x,y)\bigr)\,dxdy\end{aligned} \tag{2.16}$$

with an arbitrary ρ and any $\nu \leqslant 0$, $W = V - |x|^{-1} * \rho$.

§3. Semiclassical methods

We will need the following semiclassical expressions:

$$P'(w) = (2\pi)^{-3} q \int\limits_{\{\xi : b(\xi)\leqslant w\}} d\xi \tag{3.1}$$

and its integral

$$P(w) = (2\pi)^{-3} q \int\limits_{\{\xi : b(\xi)\leqslant w\}} b(\xi)\,d\xi, \tag{3.2}$$

where in the nonrelativistic case $b(\xi) = \frac{\hbar^2}{2\mu}|\xi|^2$ and, correspondingly for $\mu = \hbar = 1$,

$$P^{\mathsf{TF}\,\prime}(w) = \frac{q}{6\pi^2} w_+^{\frac{3}{2}}, \tag{3.3}$$

$$P^{\mathsf{TF}}(w) = \frac{q}{15\pi^2} w_+^{\frac{5}{2}}, \tag{3.4}$$

while in the relativistic case $b(\xi) = (c^2\hbar^2|\xi|^2 + \mu^2c^4)^{\frac{1}{2}} - \mu c^2$ and, correspondingly for $\mu = \hbar = 1$,

$$P^{\mathsf{RTF}\,\prime}(w) = \frac{q}{6\pi^2} w_+^{\frac{3}{2}}(1 + \beta^2 w_+)^{\frac{3}{2}}. \tag{3.5}$$

Note that $P^{\mathsf{RTF}}(w)$ is an elementary function as well, and a sadistic Calculus instructor can give it on the test. However it turns out that we really do not need any separate relativistic Thomas–Fermi theory.

After scalings we have a *semiclassical zone* $\mathcal{X}_{\mathsf{scl}} := \{x\colon \ell(x) \geqslant cZ^{-1}\}$, where the effective semiclassical parameter is $h = 1/\zeta\ell$. Then, from the semiclassical point of view, on the energy levels $\leqslant 0$, the relativistic operator has the same properties as the nonrelativistic one.

There is also a *singular zone* $\mathcal{X}_{\mathsf{sing}} =: \{x\colon \ell(x) \leqslant cZ^{-1}\}$ and it covers the *relativistic zone* $\mathcal{X}_{\mathsf{rel}} =: \{x\colon \ell(x) \leqslant c\beta\}$. The important properties are that

$$0 \leqslant V(x) - W(x) \leqslant C\zeta^2 =: \min(Z^{\frac{4}{3}}, Z\ell^{-1}), \tag{3.6}$$

$$|\partial^\gamma (W - V)| \leqslant C\zeta^2 \ell(x)^{-|\gamma|} \quad \text{for all} \quad \gamma : |\gamma| \leqslant 2. \tag{3.7}$$

3.1. Trace term. Now the rescaling methods of [9] allow us to prove the following statement.

Proposition 9. *Let condition* (1.8) *be fulfilled, and let W satisfy* (3.6) *and* (3.7).

(1) *Let $\psi_0(x)$ be an ℓ-admissible function*[3] *equal to* 1 *in* $\{x\colon \ell(x) \geqslant 2a\}$ *and supported in* $\{x\colon \ell(x) \geqslant a\}$. *Then for $W = W^{\mathsf{TF}}$ we have*

$$\Bigl|\mathrm{Tr}(H^-_{W+\lambda}\psi_0) - \int P^{\mathsf{RTF}}(W+\lambda)\psi_0(x)\,dx\Bigr| \leqslant C\begin{cases} Z^{\frac{3}{2}}a^{-\frac{1}{2}}, & a\leqslant Z^{-\frac{1}{3}},\\ Z^{\frac{5}{3}}(aZ^{\frac{1}{3}})^{-\delta}, & a\geqslant Z^{-\frac{1}{3}}.\end{cases} \tag{3.8}$$

(2) *Let $\psi_m(x)$ be ℓ-admissible, equal to* 1 *in* $\{x\colon |x - \mathsf{y}_m| \leqslant a\}$, *and supported in* $\{x\colon |x - \mathsf{y}_m| \leqslant 2a\}$. *Then for $W = V_m = Z_m|x - \mathsf{y}_m|^{-1}$ we have*

$$\Bigl|\int \bigl(\mathrm{tr}(e^1(x,x,0)) - P^{\mathsf{RTF}}(V_m)\bigr)(1 - \psi_m(x))\,dx\Bigr| \leqslant Z^{\frac{3}{2}}d^{-\frac{1}{2}}, \tag{3.9}$$

where $e^1(\,\cdot\,,\,\cdot\,,\tau) = \int_{-\infty}^{\tau} e(\,\cdot\,,\,\cdot\,,\tau')\,d\tau'$.

Proof. Indeed, the contribution of the ℓ-element of the partition[4] to the remainder is $O(\zeta^3\ell)$, exactly as in the nonrelativistic case. Summation by partition elements results in the right-hand expression. □

Next, we need to consider vicinities of the singularities. The methods of Chapter 25 of [9] allow us to prove the following.

Proposition 10. *In the framework of Proposition* 9. *let ϕ_m be equal to* 1 *in* $\{x\colon |x-\mathsf{y}_m| \leqslant Z_m^{-1}\}$ *and supported in* $\{x\colon |x-\mathsf{y}_m| \leqslant 2Z_m^{-1}\}$. *Let* $|\lambda| \leqslant C_0Zd^{-1}$.

[3] I.e., $\partial^\alpha\psi_0| \leqslant C_\alpha \ell^{-\alpha}$.

[4] I.e., an ℓ-admissible function $\psi(x)$ supported in $\frac{1}{2}\ell(y)$ for some y; then $\ell(x) \asymp \ell(y)$ on $\mathrm{supp}(\psi)$.

Then

$$\begin{gathered}\Bigl|\operatorname{Tr}(H^-_{W+\lambda}\psi_m(1-\phi_m)) - \operatorname{Tr}(H^-_{V_m}\psi_m(1-\phi_m))\\ + \int \bigl(P^{\mathsf{RTF}}(W+\lambda) - P^{\mathsf{RTF}}(V_m)\bigr)\psi_m(x)(1-\phi_m(x))\,dx\Bigr|\\ \leqslant C\begin{cases} Z^{\frac{3}{2}}d^{-\frac{1}{2}}, & d\leqslant Z^{-\frac{1}{3}},\\ Z^{\frac{5}{3}}, & d\geqslant Z^{-\frac{1}{3}},\end{cases}\end{gathered}\tag{3.10}$$

where $d \geqslant cZ^{-1}$ *is the minimal distance between nuclei.*

Proof. Indeed, exactly as in the nonrelativistic case, using methods of Sections 12.5 and 25.4 of [9], we estimate the contribution of an ℓ-element to the remainder by $O(\zeta\ell^3\bar\zeta^2\bar\ell^{-2})$ provided $Z^{-1+\delta} \lesssim \ell \lesssim d$, and by $O(\zeta^2\ell^2\bar\zeta^2)$ provided $Z^{-1} \lesssim \ell \lesssim Z^{-1+\delta}$. Here $\bar\ell = d$ and $\bar\zeta = Z^{\frac{1}{2}}d^{-\frac{1}{2}}$. This proves the required remainder estimate. For $d \leqslant Z^{-1+\delta}$ we use a rescaling.

Summation by partition elements results in the right-hand expression. □

Remark 11. We need to include the cut-off $(1-\phi_m(x))$ because not only integrals of $P^{\mathsf{RTF}}(W+\lambda)$ and $P^{\mathsf{RTF}}(V_m)$ (of magnitude $\beta^3Z^4\ell^{-4}$) and $P^{\mathsf{RTF}\,\prime}(W+\lambda)$ diverge at y_m, but even the integral of their difference diverges logarithmically.

Now we need to consider the CZ^{-1} vicinities of y_m and we will use the following proposition.

Proposition 12. *In the framework of Proposition* 9*, we have*

(i) $H_W \geqslant -C_0Z^2$*;*

(ii) *next,*

$$e(x,x,\lambda) \leqslant CZ^{1-\delta}\ell(x)^{\delta-2} \qquad \textit{for}\ \ |\lambda| \leqslant c_0Z^2. \tag{3.11}$$

Proof. (a) Assume first that $Z \asymp \beta^{-1}$ (i.e., $Z \geqslant \epsilon_0\beta^{-1}$); then Proposition 12 follows immediately from the Lieb–Yau inequality (Theorem 28): in the operator sense we have

$$H \geqslant \beta^{-1}\sqrt{\Delta} - \beta^{-2} - Z_mr^{-1} \geqslant -\beta^{-2}, \quad r = |x-\mathsf{y}_m|.$$

Then $e(x,x,\lambda) \leqslant C\ell(x)^{-3}h^{-3}$ with the semiclassical parameter h, which is $\asymp 1$ for $\ell \lesssim Z^{-1}$, $\lambda \lesssim Z^2$. Therefore,

$$e(x,x,\lambda) \leqslant C\ell(x)^{-3} \qquad \text{for}\ \ \lambda \leqslant C_0Z^2,\ \ell(x) \lesssim Z^{-1}. \tag{3.12}$$

Unfortunately, this estimate falls short for our needs. Let us shift $\mathsf{y}_m \mapsto 0$, and scale $x \mapsto Zx$, $\tau \mapsto Z^{-2}\tau$. Then we arrive at an operator that is $\sqrt{\Delta} - Zr^{-1}$ modulo $O(1)$. Since

$$\sqrt{\Delta} - \frac{2}{\pi|x|} \geqslant A_s(\Delta)^s - B_s \tag{3.13}$$

for any $s \in [0, 1/2)$ and $A_s, B_s > 0$, we can "trade" (due to Sobolev embedding theorem) $\ell^{-1+\delta}$ by 1 in the scaled inequality (3.12) and by $Z^{1-\delta}$ in the original one, thus arriving at (3.11).

(b) Let us consider $Z \leqslant \epsilon_0 \beta^{-1}$. Observe that, in the operator sense,

$$H \geqslant (\frac{1}{4}\beta^{-2}r^{-2} + \beta^{-4})^{1/2} - Zr^{-1} - C\beta^{-2} \geqslant CZ^{-2};$$

the last inequality is proved separately for $r \lesssim \beta$ and for $r \gtrsim \beta$.

Moreover, we get $H \geqslant \epsilon_1 \min(r^{-2}, \beta^{-1}r^{-1})$ for $r \leqslant \epsilon_1 Z^{-1}$ and then we can trade ℓ^{-3} to CZ^3 arriving even to a stronger version of (3.12):

$$e(x, x, \lambda) \leqslant CZ^3. \tag{3.14}$$

Actually estimate (3.14) holds as $Z_m\beta \leqslant 2\pi^{-1} - \sigma$ for $\sigma > 0$, with $C = C(\sigma)$ that could be calculated explicitly. □

Then we immediately observe the following.

Corollary 13. *In the framework of Proposition* 9*, for* $|\lambda| \leqslant C_0 Z d^{-1}$ *we have*

$$|\operatorname{Tr}(H^-_{W+\lambda}\phi_m) - \operatorname{Tr}(H^-_{V_m}\phi_m)| \leqslant CZd^{-1}. \tag{3.15}$$

Now we can assemble all these results. However, before doing this we replace P^{RTF} by P^{TF}.

Proposition 14. (1) *Estimates* (3.8)*,* (3.9)*, and* (3.10) *are true with* P^{RTF} *replaced by* P^{TF}*.*

(2) *Estimate* (3.10) *with* P^{RTF} *replaced by* P^{TF} *is also true with* $\phi_m = 0$*.*

Proof. Statement 1 follows immediately from the relations

$$\begin{aligned} &P^{\mathsf{RTF}}(w) - P^{\mathsf{TF}}(w) \asymp \beta^2 w^{\frac{7}{2}},\\ &P^{\mathsf{RTF}\,\prime}(w) - P^{\mathsf{TF}\,\prime}(w) \asymp \beta^2 w^{\frac{5}{2}} \quad \text{for } \beta^2 w \lesssim 1 \end{aligned} \tag{3.16}$$

due to (3.5). Statement 2 is an immediate consequence of

$$P^{\mathsf{TF}}(w) \asymp w^{\frac{5}{2}}, \quad P^{\mathsf{TF}\,\prime}(w) \asymp w^{\frac{3}{2}}.$$

□

Remark 15. Meanwhile,

$$\int \bigl(P^{\mathsf{RTF}}(V+\lambda) - P^{\mathsf{TF}}(V+\lambda)\bigr)\psi(x)\,dx \asymp \beta^2 Z^4, \tag{3.17}$$

which could be as large as Z^2.

Due to the scaling properties of $e(x, x, 0)$ for $H = H_V$ and $P^{\mathsf{TF}}(V)$ for $V = V_m$ we conclude that

$$\int \bigl(\operatorname{tr}(e^1(x, x, 0)) - P^{\mathsf{RTF}}(V_m)\bigr)\,dx = qZ_m^2 S(Z_m\beta) \tag{3.18}$$

with an unknown function $S(Z_m\beta)$. Indeed, if $\mathsf{y}_m = 0$, then $x \mapsto x/k$ transforms the operator with the parameters Z_m, β into the operator with the parameters $Z_m k$, βk^{-1}, multiplied by k^{-2}.

Remark 16. Obviously, $S(Z_m\beta)$ is monotone decreasing as $\beta \to 0+$ and tends to $S(0)$ for the Schrödinger operator.

Then by (3.9) for $V = V_m$ we have

$$\Bigl|\int \bigl(\operatorname{tr}(e^1(x,x,0)) - P^{\mathsf{TF}}(V_m)\bigr)\psi_m(x)\,dx - qZ_m^2 S(Z_m\beta)\Bigr| \leqslant Z^{\frac{3}{2}}d^{-\frac{1}{2}} \tag{3.19}$$

and we arrive at the next statement.

Proposition 17. *Let* (1.8) *be fulfilled. Then for* $W = W^{\mathsf{TF}}$ *we have*

$$\begin{aligned} |\operatorname{Tr}(H^-_{W+\lambda}) + \int P^{\mathsf{TF}}(W+\lambda)\,dx - \sum_{1\leqslant m\leqslant M} qZ_m^2 S(Z_m\beta)| \\ \leqslant C\begin{cases} Z^{\frac{3}{2}}d^{-\frac{1}{2}}, & d \leqslant Z^{-\frac{1}{3}}, \\ Z^{\frac{5}{3}}, & d \geqslant Z^{-\frac{1}{3}}. \end{cases} \end{aligned} \tag{3.20}$$

3.2. Trace term. II. We improve the above results for $d \gg Z^{-\frac{1}{3}}$. First, we observe that the in this case the error in (3.8) can be made

$$O\Bigl(Z^{\frac{5}{3}}\bigl(dZ^{\frac{1}{3}}\bigr)^{-\delta} + Z^{\frac{5}{3}-\delta}\Bigr),$$

provided we include the relativistic Schwinger correction term. Since this term has magnitude $Z^{\frac{5}{3}}$ and the contributions of the zones $\{x\colon \ell(x) \leqslant Z^{-\frac{1}{3}-\delta_1}\}$ and $\{x\colon \ell(x) \geqslant Z^{-\frac{1}{3}+\delta_1}\}$ in this term are $O(Z^{\frac{5}{3}-\delta})$, the difference between the relativistic and the standard nonrelativistic Schwinger terms is $O(Z^{\frac{5}{3}-\delta})$, and we can use the latter,

$$\mathsf{Schwinger} = (36\pi)^{\frac{2}{3}} q^{\frac{2}{3}} \int \bigl(\rho^{\mathsf{TF}}\bigr)^{\frac{4}{3}}\,dx. \tag{3.21}$$

Next, consider the relativistic correction term

$$\int\Bigl(-P^{\mathsf{RTF}}(W+\lambda)+P^{\mathsf{RTF}}(V_m)+P^{\mathsf{TF}}(W+\lambda)-P^{\mathsf{TF}}(V_m)\Bigr)\psi_m(1-\phi_m)\,dx. \tag{3.22}$$

Again, it can easily be seen that we need to consider only the contribution of the *threshold zone* $\mathcal{Y} \coloneqq \{x\colon Z^{-\frac{1}{3}-\delta_1} \leqslant \ell(x) \leqslant Z^{-\frac{1}{3}+\delta_1}\}$, because the contributions of the two zones $\{x\colon \ell(x) \leqslant Z^{-\frac{1}{3}-\delta_1}\}$ and $\{x\colon \ell(x) \geqslant Z^{-\frac{1}{3}+\delta_1}\}$ to this term are $O(Z^{\frac{5}{3}-\delta})$.

It is easy to show that in the threshold zone, by (3.5),

$$P^{\mathsf{RTF}}(w) - P^{\mathsf{TF}}(w) = \frac{q}{14\pi^2}\beta^2 w_+^{\frac{7}{2}} + O\bigl(Z^{\frac{8}{3}-\delta}\bigr)$$

(for both $w = W^{\mathsf{TF}} + \lambda$ and $w = V_m$), and therefore, modulo the same error expression, (3.22) coincides with

$$\mathsf{RCT} =: \frac{q}{14\pi^2}\beta^2 \int \bigl(-(W^{\mathsf{TF}} + \lambda)_+^{\frac{7}{2}} + V^{\frac{7}{2}}\bigr)\, dx \tag{3.23}$$

with the integral taken over this zone or $\mathbb{R}^3$ (it does not matter). We arrive at the following statement.

Proposition 18. *Suppose* (1.8) *is fulfilled and* $d \geqslant Z^{-\frac{1}{3}}$. *Then for* $W = W^{\mathsf{TF}}$ *we have*

$$\begin{aligned} |\operatorname{Tr}(H^-_{W+\lambda}) + \int P^{\mathsf{TF}}(W+\lambda)\, dx - \sum_{1\leqslant m\leqslant M} qZ_m^2 S(Z_m\beta) - \mathsf{Schwinger} - \mathsf{RCT}| \\ \leqslant C\bigl(Z^{\frac{5}{3}}(dZ^{\frac{1}{3}})^{-\delta} + Z^{\frac{5}{3}-\delta}\bigr). \end{aligned} \tag{3.24}$$

3.3. Trace term. III. Obviously, all these results are valid for $W = W_\varepsilon$ defined by (2.14) with $\rho = \rho^{\mathsf{TF}}$. However, we need to estimate an error when we replace W_ε by W^{TF}. It is easy to prove that

$$|W_\varepsilon - W^{\mathsf{TF}}| \leqslant C_s (Z\ell^{-1})^{\frac{3}{2}} \varepsilon^2 (\varepsilon\ell{-}1)^s \tag{3.25}$$

with arbitrary s for $\ell \leqslant \epsilon_0 Z^{-\frac{1}{3}}$ and with $s = \frac{1}{2}$ for $\ell \leqslant \epsilon_0 Z^{-\frac{1}{3}}$, and therefore,

$$\Bigl|\int \bigl(P^{\mathsf{TF}}(W_\varepsilon + \lambda) - P^{\mathsf{TF}}(W^{\mathsf{TF}} + \lambda)\, dx\Bigr| \leqslant CZ^3\varepsilon^2. \tag{3.26}$$

Adding an error of $CZ\varepsilon^{-1}$ in (2.15), we get $C(Z^3\varepsilon^2 + Z\varepsilon^{-1})$. It attains its minimum $CZ^{\frac{5}{3}}$ as $\varepsilon \asymp Z^{-\frac{2}{3}}$ and we arrive at the next claim.

Proposition 19. *Let* (1.8) *be fulfilled. Then for* $W = W_\varepsilon$ *with* $\varepsilon = Z^{-\frac{2}{3}}$, (3.20) *holds true, and the left-hand expression in* (3.26) *is* $O(Z^{\frac{5}{3}})$.

3.4. N- and D-terms. For these terms (needed for the estimate from above) arguments are simpler; let $\phi_0 = 1 - \phi_1 - \cdots - \phi_M$.

Proposition 20. *In the framework of Proposition 9,*

(i) *we have*

$$\Bigl|\int \bigl(e(x,x,\lambda)-P^{\mathsf{RTF}\,\prime}(W+\lambda)\bigr)\phi_0(x)\,dx\Bigr|\leqslant CZ^{\frac{2}{3}},\tag{3.27}$$

and for $d\geqslant Z^{-\frac{1}{3}}$

$$\Bigl|\int \bigl(e(x,x,\lambda)-P^{\mathsf{RTF}\,\prime}(W+\lambda)\bigr)\phi_0(x)\,dx\Bigr|\leqslant C\Bigl(Z^{\frac{2}{3}}(dZ^{\frac{1}{3}})^{-\delta}+Z^{\frac{2}{3}-\delta}\Bigr);\tag{3.28}$$

(ii) *next,*

$$\Bigl|\int e(x,x,\lambda)\phi_m(x)\,dx\Bigr|\leqslant C;\tag{3.29}$$

(iii) *and finally,*

$$\Bigl|\int \bigl(P^{\mathsf{RTF}\,\prime}(W+\lambda)-P^{\mathsf{TF}\,\prime}(W+\lambda)\bigr)\phi_0(x)\,dx\Bigr|\leqslant CZ^{\frac{1}{3}}.\tag{3.30}$$

Proposition 21. *In the framework of Proposition 9,*

(i) *we have*

$$\begin{aligned}\mathsf{D}\Bigl(\bigl(e(x,x,\lambda)-P^{\mathsf{RTF}\,\prime}(W+\lambda)\bigr)\phi_0,&\\ \bigl(e(x,x,\lambda)-P^{\mathsf{RTF}\,\prime}(W+\lambda)\bigr)\phi_0\Bigr)&\leqslant CZ^{\frac{5}{3}},\end{aligned}\tag{3.31}$$

and for $d\geqslant Z^{-\frac{1}{3}}$

$$\begin{aligned}\mathsf{D}\Bigl(\bigl(e(x,x,\lambda)-P^{\mathsf{RTF}\,\prime}(W+\lambda)\bigr)\phi_0,&\\ \bigl(e(x,x,\lambda)-P^{\mathsf{RTF}\,\prime}(W+\lambda)\bigr)\phi_0\Bigr)&\leqslant CZ^{\frac{5}{3}}\bigl(dZ^{\frac{1}{3}}\bigr)^{-\delta}+CZ^{\frac{5}{3}-\delta};\end{aligned}\tag{3.32}$$

(ii) *next,*

$$\mathsf{D}\bigl(e(x,x,\lambda)\phi_m(x),\,e(x,x,\lambda)\phi_m(x)\bigr)\leqslant CZ;\tag{3.33}$$

(iii) *and finally,*

$$\begin{aligned}\mathsf{D}\Bigl(\bigl(P^{\mathsf{RTF}\,\prime}(W+\lambda)-P^{\mathsf{TF}\,\prime}(W+\lambda)\bigr)\phi_0,&\\ \bigl(P^{\mathsf{RTF}\,\prime}(W+\lambda)-P^{\mathsf{TF}\,\prime}(W+\lambda)\bigr)\phi_0\Bigr)&\leqslant CZ.\end{aligned}\tag{3.34}$$

Proof of Propositions 20 and 21. The proof is straightforward:

Statements (i) are proved by the semiclassical scaling technique exactly as in [9, Chapter 25].

Statements (ii) follow from Proposition 12. Statements (iii) follow from (3.5) and the properties of W^{TF}. □

3.5. Dirac term. Finally, consider the term

$$-\frac{1}{2}\iint \operatorname{tr}\bigl(e_N^\dagger(x,y)e_N(x,y)\bigr)\,dxdy.$$

The main contribution to it is delivered by the zone $\mathcal{Y}\times\mathcal{Y}$, where $\mathcal{Y}$ is the threshold zone, and in this zone the nonmagnetic approximation delivers the correct expression

$$\mathsf{Dirac} = -\frac{9}{2}(36\pi)^{\frac{2}{3}}q^{\frac{2}{3}}\int (\rho^{\mathsf{TF}})^{\frac{4}{3}}\,dx, \tag{3.35}$$

with an error of $Z^{\frac{5}{3}-\delta}$.

§4. Main theorems

Now, repeating the arguments of [9, Section 25.4] we arrive to our main results.

Theorem 22. [5] *Let assumption* (1.8) *be fulfilled.*

(i) *We have the following asymptotics*:

$$\mathsf{E}_N = \mathcal{E}_N^{\mathsf{TF}} + \mathsf{Scott} + O\bigl(Z^{\frac{5}{3}} + Z^{\frac{3}{2}}d^{-\frac{1}{2}}\bigr). \tag{4.1}$$

Recall that $\mathsf{Scott} = q\sum Z_m^2 S(Z_m\beta)$ *and* d *is the minimal distance between the nuclei.*

(ii) *Furthermore, let assumption* (1.9) *be fulfilled. Then for* $d \geqslant Z^{-\frac{1}{3}}$ *we have*

$$\mathsf{E}_N = \mathcal{E}_N^{\mathsf{TF}} + \mathsf{Scott} + \mathsf{Dirac} + \mathsf{Swinger} + \mathsf{RCT} + O\Bigl(Z^{\frac{5}{3}}\bigl(dZ^{\frac{1}{3}}\bigr)^{-\delta} + Z^{\frac{5}{3}-\delta}\Bigr). \tag{4.2}$$

Remark 23. (i) For the improved upper estimate in (4.2) we do not need the assumption (1.9).

(ii) These theorems allow us to consider the free nuclei model and recover Theorem 25.4.14 of [9], albeit without assumption (1.9) we get only $\delta = 0$.

(iii) We also recover the estimate

$$|\lambda_N - \nu| \leqslant C\begin{cases} Z^{\frac{8}{9}} & \text{if } \ (Z-N)_+ \leqslant Z^{\frac{2}{3}},\\ (Z-N)_+^{\frac{1}{3}} & \text{if } \ (Z-N)_+ \geqslant Z^{\frac{2}{3}}, \end{cases} \tag{4.3}$$

where ν is a chemical potential and λ_N is the Nth lowest eigenvalue of $H_{W^{\mathsf{TF}}}$ (reset to 0 if there are less than N negative eigenvalues). Furthermore, for $d \geqslant Z^{-\frac{1}{3}}$ one can include the factor $((dZ^{\frac{1}{3}})^{-\delta} + Z^{-\delta})$ into the right-hand expression.

[5] Cf. Theorems 25.4.8 and 25.4.13 in [9].

Theorem 24. [6] *Let assumption* (1.9) *be fulfilled. Then*:

(i) *we have*
$$\mathsf{D}(\rho_\Psi-\rho^{\mathsf{TF}},\,\rho_\Psi-\rho^{\mathsf{TF}})\leqslant CZ^{\frac{5}{3}};\tag{4.4}$$

(ii) *furthermore, for* $d\geqslant Z^{-\frac{1}{3}}$,
$$\mathsf{D}\bigl(\rho_\Psi-\rho^{\mathsf{TF}},\,\rho_\Psi-\rho^{\mathsf{TF}}\bigr)\leqslant C\bigl(Z^{\frac{5}{3}}\bigl(dZ^{\frac{1}{3}}\bigr)^{-\delta}+Z^{\frac{5}{3}-\delta}\bigr).\tag{4.5}$$

Remark 25. (i) Estimates (4.4) and (4.5) allow us to consider the excessive negative charge and ionization energy and, repeating arguments of [9, Section 25.5], to recover Theorems 25.5.2 and 25.5.3.

(ii) Further, these estimates allow us to consider the excessive positive charge in the free nuclei model and, repeating arguments of [9, Section 25.6], to recover Theorems 25.6.3 and 25.6.4.

Remark 26. We can even make a poor man version of (4.2) in the critical case, when only assumption (1.8) is fulfilled.

(i) Consider how our terms depend on q. In the atomic case consider given Z, N and shift to $\mathsf{y}_1=0$. Then
$$\rho_q^{\mathsf{TF}}(x)=q^2\rho_1^{\mathsf{TF}}(q^{\frac{2}{3}}x),\qquad W_q^{\mathsf{TF}}(x)=q^{\frac{2}{3}}W_1^{\mathsf{TF}}(q^{\frac{2}{3}}x),\tag{4.6}$$
and $\mathcal{E}^{\mathsf{TF}}\asymp q^{\frac{2}{3}}Z^{\frac{7}{3}}$, $\mathsf{Scott}\asymp qZ^2$, $\mathsf{Dirac}\asymp\mathsf{Schwinger}\asymp q^{\frac{4}{3}}Z^{\frac{5}{3}}$, while $\mathsf{RCT}\asymp q^{\frac{4}{3}}\beta^2Z^{\frac{11}{3}}$.

(ii) Repeating the corresponding arguments in [13], one can prove that in the correlation inequality (2.13), the constant is $C(q)\leqslant C_0q^{\frac{2}{3}}$. On the other hand, we use the estimate for $|W-W_\varepsilon|\asymp q\varepsilon^2Z^{\frac{3}{2}}\ell^{-\frac{3}{2}}$ and then the approximation error is $C_0Z^3q^2\varepsilon^2$. Optimizing $Z^3q^2\varepsilon^2+Zq^{\frac{2}{3}}\varepsilon^{-1}$ in ε, we get $Cq^{\frac{10}{9}}Z^{\frac{5}{3}}$ and for a large constant q it is less than $q^{\frac{4}{3}}$. In the "real life" $q=2$.

§5. Appendix: Some inequalities

We follow [13] with some modifications:

We recall that the following two inequalities are crucial in many of our estimates. They serve as replacements for the Lieb–Thirring inequality [11] used in the nonrelativistic case.

Theorem 27 (Daubechies inequality). (i) *One-body case*:
$$\operatorname{Tr}\bigl[(\beta^{-2}\Delta+\beta^{-4})^{\frac{1}{2}}-\beta^{-2}-V(\mathsf{x})\bigr]^-\geqslant -C\int\Bigl(V_+^{(n+2)/2}+\beta^nV_+^{n+1}\Bigr)\,dx.\tag{5.1}$$
where $n\geqslant 3$ *is a dimension.*

[6] Cf. Theorem 25.4.15 in [9].

(ii) Many-body case: *Let* $\Psi \in \bigwedge_{j=1}^{N} \mathscr{L}^2(\mathbb{R}^3;\mathbb{C}^q)$, *and let* ρ_Ψ *be its one-particle density. Then for* $n=3$ *we have*

$$\Big\langle \sum_{j=1}^{N} \Big[\big(\beta^{-2}\Delta_j + \beta^{-4}\big)^{\frac{1}{2}} - \beta^{-2} \Big] \Psi, \Psi \Big\rangle \geqslant \int \min\Big(\rho_\Psi^{\frac{5}{3}}, \beta^{-1}\rho_\Psi^{\frac{4}{3}}\Big)\, dx. \tag{5.2}$$

This theorem is also valid in the nonrelativistic limit $\beta = 0$ with the operator $(\beta^{-2}\Delta + \beta^{-4})^{\frac{1}{2}} - \beta^{-2}$ replaced by $\frac{1}{2}\Delta$.

Theorem 28 (Lieb–Yau inequality). *Let* $n = 3$. *Suppose* $C > 0$ *and* $R > 0$, *and let*

$$H_{C,R} = \Delta^{\frac{1}{2}} - \frac{2}{\pi|x|} - C/R. \tag{5.3}$$

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

$$\mathrm{Tr}\big[\bar{\theta}\gamma\theta H_{C,R}\big] \geqslant -4.4827\, C^4 R^{-1} \Big\{ 3/(4\pi R^3) \int |\theta(x)|^2\, dx \Big\}. \tag{5.4}$$

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

Theorem 29 (Critical Hydrogen inequality). *Let* $n = 3$. *For any* $s \in [0, 1/2)$ *there exists constants* $A_s, B_s > 0$ *such that*

$$\Delta^{\frac{1}{2}} - \frac{2}{\pi|x|} \geqslant A_s \Delta^s - B_s. \tag{5.5}$$

Theorem 30 (Hardy–Littlewood–Sobolev inequality). *There exists a constant* C *such that*

$$\mathsf{D}(f) =: \iint |x-y|^{-1} f(x) f^\dagger(y)\, dx dy \leqslant C\, \|f\|^2_{\mathscr{L}^{6/5}}. \tag{5.6}$$

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