The Semiclassical Limit of Thomas–Fermi Theory Forty Years After

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My work with Elliott Lieb on TF theory was stretched out some, starting in the fall of 1972 with the final publication of the long paper on the subject only in 1977, but it is fair to say that the key step, where we knew we had a large $\mathbb{Z}$ limit theorem for atoms, took place in March 1973 (when we “pulled the Poisson Coulomb tooth”), so this year is the 40th anniversary of this work.
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In the fall of 1972, we were both visiting IHES near Paris. Elliott was forty—recently hired by MIT after the splash of his work on six vertex models (and the entropy of square ice), written while he was at Boston University.
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Elliott and I started talking a lot and, early on, he suggested we look at Thomas–Fermi theory, which he felt should be exact in the large $Z$-limit.
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Arthur passed away last January (at age 90), and I want to acknowledge my huge personal debt to him as well as the debt of the mathematical physics community.
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Arthur included a week on Thomas–Fermi theory, including Teller’s Theorem that atoms don’t bind in TF theory.
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So Teller’s Theorem is irrelevant to the $Z \to \infty$ limit result although, of course, as Lieb and Thirring realized a few years later, it was very relevant to the stability of matter!
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3. Dealing with the Strong Coulomb Singularity
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In March, I went from Marseille to Paris where Elliott had an apartment for the year. We banged our heads on the Coulomb singularity for several days and finally solved the problem.
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Thomas and Fermi described their equation for the electron density $\rho$ by supposing they were in a semiclassical limit where the local momentum of a particle at the top of the Fermi sphere was $p_F(x) = cr(x)$ while $\rho(x) = dr(x)^3$ so $p_F^2 = c_1 \rho(x)^{2/3}$. The potential energy is given by
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$$\varphi(x) = V(x) - \int \rho(x)|x - y|^{-1} dy$$
Existence Problems

Constancy of the Fermi energy required

\[(2m)^{-1}p_F^2 - \varphi(x) = \varphi_0 \quad \text{(at points when } \rho > 0)\]
\[\geq \varphi_0 \quad \text{(at points when } \rho \geq 0)\]
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So they got a self-consistent non-linear integral equation

\[c \rho^{2/3}(x) = (V(x) - \int |x - y|^{-1} \rho(y)dy - \varphi_0)_+\]
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If \(V(x)\) is Coulomb with charges at \(R_1, \ldots, R_k\), then for \(x \notin \{R_1, \ldots, R_k\}\), \(\varphi\) obeys

\[\Delta \varphi = c(\varphi - \varphi_0)^{3/2}\]
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Hille also rigorously proved in the spherically symmetric neutral case ($\varphi_0 = 0$), $\rho_{TF}(x) \sim Cx^{-6}$, something computed by Sommerfeld in 1932.
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As a bonus, \( \rho = \delta \mathcal{E} / \delta V \) so we could get convergence of derivatives using the miracle of convex functions.
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Also fortunately, as a graduate student at Princeton, I’d take a course given by Choquet (the basis of his book by Marsden et al., also students in the course) and he’d used a tool which was exactly what we needed!
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Elliott is, of course, now a leading figure in subtle uses of the direct method. I’m pleased if I helped provide his initial exposure to this subject.
After completing existence and the quantum limit theorem, Elliott and I wrote up an announcement and sent it off to PRL (= Physical Review Letters).
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I was eventually wont to say PRL stands for Physical Review Lottery since the refereeing is so uneven. This paper is part of that story.
Fun and Games with Papers

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The paper took a while to write, since after our joint European jaunt, Elliott returned to MIT and I returned to Princeton. But then we lured Elliott to Princeton and things went faster. We submitted it to *Advances in Mathematics*, which solicited it and then sat on it for two years.
We fix $z_1, \ldots, z_\ell \geq 0$ and $R_1, \ldots, R_\ell$ and let

$$V(x; z_1, \ldots, z_\ell; R_1, \ldots, R_\ell) = \sum \frac{z_j}{|r - R_j|}$$

and

$$\mathcal{E}_{TF}(\rho, V) = \frac{3}{5} \int \rho(x)^{5/3} d^3 x - \int V(x)\rho(x) d^3 x + \frac{1}{2} \int \int \frac{\rho(x)\rho(y)}{|x - y|} d^3 x d^3 y$$
Existence of Solutions

We fix \( z_1, \ldots, z_\ell \geq 0 \) and \( R_1, \ldots, R_\ell \) and let

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We pick the set of trial functions

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Since $|x|^{-1} \in L^{5/2} + L^\infty$, each term in $\mathcal{E}_{TF}$ is well defined if $\rho \in \mathcal{T}$.
Existence of Solutions

**Theorem 1.** For any $N$, there is a unique $\rho \in \mathcal{T}$ minimizing \( \{ \mathcal{E}(\rho) \mid \rho \in \mathcal{T}, \int \rho(x)d^3x \leq N \} \).
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This follows from strict convexity and the direct method and the fact that $\{\rho \in \mathcal{T} \mid \int \rho d^3x \leq N\}$ is weakly closed. (Note: $\{\rho \in \mathcal{T} \mid \int \rho d^3x = N\}$ is not.)
No Negative Ions in TF Theory

**Theorem 2.** If $N \leq Z = \sum_{j=1}^{\ell} z_j$, then the minimizer has $\int \rho \, d^3x = N$. If $N > Z$, the minimizer has $\int \rho \, d^3x = Z$. The minimizer for $N = Z$ is a minimizer over all of $\mathcal{T}$. 
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The proof depends on noting the minimizer obeys

$$\rho^{2/3}(x) = (\varphi(x) - \varphi_0)^+$$

$$\varphi(x) = V(x) - \int \frac{\rho(y)}{|x - y|} \, d^3y$$
\( \varphi_0 \geq 0 \) because if \( e(\lambda) = \min(\int \rho = \lambda) \), then \( \varphi_0 = -\frac{de}{d\lambda} \) and \( e \) is decreasing.
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Thus on \( \{x \mid \varphi(x) < 0\} \), \( \rho \) is zero so \( \varphi \) is harmonic. Given that \( \varphi \to 0 \) at \( \infty \), we conclude \( \varphi \) must be non-negative since otherwise it would have a minimum.
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But \(\int \varphi(r\omega)d\omega \sim \frac{Z-N}{r}\) for \(r\) large. If \(Z < N\), we get a contradiction.
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But \( \int \varphi(r\omega)d\omega \sim \frac{Z-N}{r} \) for \( r \) large. If \( Z < N \), we get a contradiction.

Similar arguments show the absolute minimum has to have \( Z = N \).
Properties of $\rho_{TF}$

We also proved that away from $\{R_j\}$, $\rho_{TF}$ is $C^\infty$ in the region where $\rho_{TF} \geq 0$ which is all of $\mathbb{R}^3$ when $Z = N$. 
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We proved Sommerfeld’s asymptotic formula, the first proof in the molecular case (Sommerfeld asked when \( c|x|^{-\alpha} \) solves \( \Delta \varphi = d\varphi^{3/2} \) on \( \mathbb{R}^3 \setminus \{0\} \) and found \( \alpha = 4 \) and \( c \) in terms of \( d \)).
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**Theorem 3.** The solution \( \rho_{TF} \) in the neutral case has
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|x|^{-6} \rho(x) \to 27\pi^{-3} \text{ as } |x| \to \infty.
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**Theorem 3.** The solution \( \rho_{TF} \) in the neutral case has \( |x|^{-6} \rho(x) \to 27\pi^{-3} \text{ as } |x| \to \infty \).

The proof uses subharmonic comparison theorems and the form of the exact Sommerfeld solution of the TF ODE.
We also proved

**Theorem 4.** \( E(z_1, \ldots, z_{\ell+k}; R_1, \ldots, R_{\ell+k}) \geq E(z_1, \ldots, z_{\ell}; R_j) + E(z_{\ell+1}, \ldots, z_{\ell+k}; R_j) \)

i.e., *molecules don’t bind in TF theory.*
Teller’s Theorem

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i.e., *molecules don’t bind in TF theory.*

Put more positively: TF matter is stable in the Onsager sense.

The proof followed Teller—the most important point of rigor was the existence of solutions to neutral TF.
We want to see what happens to TF theory of an atom as $Z \to \infty$, so we look at

\[ E_Z(\rho) = \frac{3}{5} \int \rho^{5/3}(x) d^3 x - Z \int \frac{\rho(x)}{|x|} d^3 x \]
\[ + \frac{1}{2} \int \int \frac{\rho(x) \rho(y)}{|x - y|} d^3 x d^3 y \]
TF Scaling

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+ \frac{1}{2} \int \int \frac{\rho(x)\rho(y)}{|x - y|} d^3x d^3y
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We make the ansatz

$$\rho_Z(x) = Z^\alpha \rho(Z^\beta x)$$
$N(\rho Z) = Z^{\alpha - 3\beta} N(\rho)$ so to keep neutrality $\alpha - 3\beta = 1$. 
TF Scaling

\[ N(\rho_Z) = Z^{\alpha-3\beta} N(\rho) \] so to keep neutrality \( \alpha - 3\beta = 1 \).

Similarly

\[ K(\rho_Z) = Z^{2\alpha/3} Z, \quad ZA(\rho_Z) = Z(Z^{\alpha-2\beta}) A(\rho) = Z^2 Z^\beta A(\rho) \]

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\[ K \sim Z^{4/3+1} = Z^{7/3}, \ Z A \sim Z^{2+1/3}, \ R \sim Z^{4-5/3} = Z^{7/3} \]
Thus $\mathcal{E}_Z(\rho_Z) = Z^{7/3}\mathcal{E}(\rho)$ for one center.
TF Scaling

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For $\ell$ centers:

$$\mathcal{E}_{TF}(\rho Z; Zz_1, \ldots Zz_\ell; Z^{-1/3} R_1, \ldots Z^{-1/3} R_\ell) = Z^{7/3}\mathcal{E}_{TF}(\rho; z_j, R_j)$$
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For $\ell$ centers:

$$E_{TF}(\rho_Z; Zz_1, \ldots Zz_{\ell}; Z^{-1/3} R_1, \ldots Z^{-1/3} R_{\ell}) = Z^{7/3} E_{TF}(\rho; z_j, R_j)$$

**Theorem 5.** If $E(z_j, R_j, N)$ is the minimum

$$E(Zz_1; Z^{-1/3} R_j; ZN) = Z^{7/3} E(z_j, R_j, N)$$

$$\rho_{TF}(x; Zz_j; Z^{-1/3} R_j; ZN) = Z^2 \rho_{TF}(Z^{1/3} x; z_j; R_j; N)$$
An interesting observation Elliott and I made is that if \( f(x) = cx^{-6} \), then \( Z^2 f(Z^{1/3} x) = f(x) \). It is important that the natural spatial scale is \( Z^{-1/3} \) and the \( Z^2 \rho(Z^{1/3} x) \) implies in a box of sizes \( Z^{-1/3} \), there are \( O(Z^2(Z^{-1/3})) = O(Z) \) electrons. This is consistent with the notion that large \( Z \) atoms are semiclassical, i.e., large number of electrons on the natural scale.
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number of electrons on the natural scale.
Quantum Limit Theorem

For $\frac{3}{5} \int \rho^{5/3}(x) d^3x$ to be semiclassical limit of the quantum kinetic energy requires a certain value of $\hbar$ and that value depends on the number of electrons allowed and the mass (as in $\hbar^2/2m$) under the Pauli principle (i.e., 2 spin states in nature!)
Quantum Limit Theorem

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By \( H_Q(z_j, R_j) \) we mean the quantum Hamiltonian

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H_Q = -\frac{\hbar^2}{2m} \sum_{k=1}^{N} \Delta_k - \sum_{k=1}^{N} \sum_{j=1}^{\ell} \frac{z_j}{|x_k - R_j|} + \sum_{1 \leq k < q \leq N} \frac{1}{|x_k - x_q|}
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as an operator on \( L^2(\mathbb{R}^{3N}; (\mathbb{C}^2)^N) \).
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$E_Q(z_j, R_j)$ is the inf of $\langle \varphi, H_Q \varphi \rangle$ over all $\varphi$ antisymmetric in $\langle x_k, \sigma_k \rangle$. 
Our main result was

**Theorem 6.** *With the above value of $\hbar$*

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\lim_{Z \to \infty} \frac{E_Q(z_j Z, R_j Z^{-1/3})}{Z^{7/3}} = E_{TF}(z_j, R_j)
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Our main result was

**Theorem 6.** *With the above value of \( \hbar \)*

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There were subsequent results on the \( O(Z^2) \) (Scott) correction by Hughes and Siedentop and \( O(Z^{5/3}) \) by Fefferman–Seco.

In this result, \( N = \lambda Z (\lambda \leq 1) \) and \( E_{TF} \) is for \( N_{TF} = \lambda \).
We also had results on electron densities (both one and $j$ particle densities, $j$ fixed—I’ll only discuss the one particle result).
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**Theorem 7.** Let $N \leq Z$. If $\rho^Q$ is the one particle density (normalized to $\int \rho^Q(x) d^3x = N$), then $Z^{-2} \rho^Q(Z^{-1/3}x)$ converges weakly (in $L^\infty$-sense) to $\rho_{TF}(x)$. 
This result is actually a simple corollary of the energy result when $Z|x|^{-1}$ is replaced by $Z|x|^{-1} + Z^{4/3}V(Z^{1/3}x)$, so $\rho^Q(x) = \delta E_Q/\delta V(x)$ after scaling.
Quantum Limit Theorem

This result is actually a simple corollary of the energy result when \( Z|\!\!x\!\!|^{-1} \) is replaced by \( Z|\!\!x\!\!|^{-1} + Z^{4/3}V(Z^{1/3}x) \), so \( \rho^Q(x) = \delta E_Q/\delta V(x) \) after scaling.

Normally, convergence of functions does not imply convergence of derivatives—we use the fact that 
\( f_n(x) \rightarrow f(x) \), all \( f_n \) convex, and \( f \) differentiable at \( x_0 \) implies \( (D^+ f_n)(x_0) \rightarrow f_n(x_0) \).
There is a classic technique used to prove the Weyl limit theorem (on number of eigenvalues in a region) which had been used by Martin, Robinson, and Tamura shortly before our work to prove WKB asymptotics for the number of negative eigenvalues of $-\frac{\hbar^2}{2m} \Delta + V$ as $\hbar \downarrow 0$ where $V \leq 0$, $C^\infty$, and goes to zero rapidly at $\infty$. 
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It relies on a beautiful subtlety of Hilbert space unbounded operator theory. Operators have a domain, \(D(A)\), and self-adjoint operators, \(A, B\), cannot have \(D(B) \supset D(A)\) and \(B \upharpoonright D(A) = A\) (\(B\) is an extension of \(A\)), unless \(B = A\).
The Magic of Quadratic Forms

If $A$ is positive and self-adjoint, $Q(A) = A^{1/2}$ and

$$\langle \varphi, A\varphi \rangle \equiv \|A^{1/2}\varphi\|^2$$

for $\varphi \in Q(A)$. 
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An interesting example is $A = -\frac{d^2}{dx^2}$ on $L^2([0,1])$ with $\varphi(0) = \varphi(1) = 0$ boundary conditions and $B = -\frac{d}{dx}$ on $L^2([0,1])$ with $\varphi'(0) = \varphi'(1) = 0$ boundary conditions. Then $Q(A) = \{\varphi \mid \varphi \text{ continuous on } [0,1] \varphi' \text{ (distributional derivatives) in } L^2 \text{ with } \varphi(0) = \varphi(1) = 0\}$.

$Q(B)$ is the same but with no boundary condition. In each case (for $C = A$ or $B$)
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\[ \langle \varphi, C\varphi \rangle = \int_0^1 |\varphi'(x)|^2\,dx \]

Thus $Q(A) \subset Q(B)$ and $B \upharpoonright Q(A) = A!$
The Magic of Quadratic Forms

We say for $A, B$ positive and self-adjoint that $A \leq B$ if and only if

$$Q(B) \subset Q(A), \quad \varphi \in Q(B) \Rightarrow \langle \varphi, B\varphi \rangle \geq \langle \varphi, A\varphi \rangle$$
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Think of $\langle \varphi, A\varphi \rangle$ being defined for all $\varphi$ but being $\infty$ if $\varphi \notin Q(A)$. Then, $B \geq A \iff \forall \varphi \langle \varphi, B\varphi \rangle \geq \langle \varphi, A\varphi \rangle$. 

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The point is that if $A \leq B$, then those eigenvalues are also ordered.
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The point is that if $A \leq B$, then those eigenvalues are also ordered.

In the above example, $\left( -\frac{d^2}{dx^2} \right)_D \geq \left( -\frac{d^2}{dx^2} \right)_N$
If $B$ is $-\Delta + V$ on $\mathbb{R}^\nu$ and we put in some $D$ b.c., then the resulting operator has a smaller form domain since $\varphi$'s are forced to vanish on the Dirichlet boundary. If we put in Neumann b.c. functions can be discontinuous across $N$ boundary, so the domain is bigger and
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$$B_N \leq B \leq B_D$$
The Semiclassical Limit

So, for example, to treat the number of negative eigenvalues of \(-\Delta + \lambda V\) when \(\lambda \to \infty\) and \(V \in C_0^\infty(\mathbb{R}^{3N})\), cover \(\text{supp}(V)\) by rectangular boxes of side \(\delta\), let \(H_-(\lambda)\) have \(N\) b.c. and \(V\) in each but replaced by its minimum, and \(H_+(\lambda)\) have \(D\) b.c. and \(V\) replaced by its max.
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Then we need only count eigenvalues in a box with constant potential $\alpha \lambda$ where $\alpha < 0$, the control $\lim (\lambda V)/\lambda^{3/2}$ and $\lim N(\lambda V)/\lambda^{3/2}$. Then take $\delta \downarrow 0$. 
The Semiclassical Limit

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Then we need only count eigenvalues in a box with constant potential $\alpha \lambda$ where $\alpha < 0$, the control $\lim (\lambda V)/\lambda^{3/2}$ and $\lim N(\lambda V)/\lambda^{3/2}$. Then take $\delta \downarrow 0$.

If $Z/|x|$ is replaced by $Z^{4/3}V(Z^{1/3}x)$ with $V$ bounded and continuous (go to 0 at $\infty$), the same argument with boxes in $\mathbb{R}^{3N}$ proves the TF limit theorem.
The Coulomb Singularity

If quantum energies went to $-\infty$ at a rate faster than $\frac{Z^7}{3}$ due to collapse into the origin (or the $R_j$ in the molecular case), these DN bracketings wouldn’t see it.
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The upper bound is fine but since $V = -\infty$ in the boxes near the $R_j$’s, we need another way to handle the lower bound.
Reduction to One Body Problem

Let

\[ V(x; R) = \begin{cases} 
    |x|^{-1} & |x| \leq R \\
    0 & |x| > R 
\end{cases} \]
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Let

\[ e_N(Z; R, \alpha) = \text{gd state energy of } H_N(Z; R, \alpha) \]

\[ H_N(Z; R, \alpha) = -\alpha \sum_{i=1}^{N} \Delta_i - Z \sum_{i=1}^{N} V(x_i; R) \]

on \( L^2(\mathbb{R}^{3N}; \mathbb{C}^{2N})_{\text{anti}} \)
If we show for each $\alpha > 0$ and

$$\lim_{\delta \downarrow 0} \lim_{Z \to \infty} \sup_{N} \left[ Z^{-7/3} \left| e_{N}(Z; \delta Z^{-1/3}, \alpha) \right| \right] = 0$$

for $H_{Q} = \tilde{H}_{Q} + H_{N}(Z; \delta Z^{-1/3} R; \alpha)$ where $\tilde{H}_{Q}$ has the Coulomb tooth pulled and $\Delta$ replaced by $(1 - \alpha)\Delta$. 
Reduction to One Body Problem

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$$E(A + B) \geq E(A) + E(B)$$

so we get a lower bound for $\alpha, \delta$ fixed on $\lim E_Q/Z^{7/3}$ by one term involving $\lim_{Z \to \infty} Z^{-7/3} e_N(Z; \delta Z^{-1/3}; \alpha)$ and one term controlled by cutoff Coulomb TF. Then take $\delta \downarrow 0$ and $\alpha \downarrow 0$. 

Reduction to One Body Problem

So we are now dealing with a one body problem! If $\lambda_j$ are the negatives ev. of $-\alpha \Delta - ZV(x; R)$, then (2 spin states)

$$|e_N| \leq 2 \sum_j \lambda_j$$
So we are now dealing with a one body problem! If \( \lambda_j \) are the negatives ev. of \(-\alpha \Delta - ZV(x; R)\), then (2 spin states)

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We proved

\[
\frac{1}{2}|e_N| \leq Z^2 \alpha^{-1} + Z^{5/2} \alpha^{-3/2} R^{1/2}
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\]

Picking \( R = \delta Z^{-1/3} \) and using \( Z^{5/2} Z^{-1/6} = Z^{7/3} \) (!) and we see

\[
|e_N(Z; \delta Z^{-1/3} \alpha)| \leq Z^2 \alpha^{-1} + \delta^{1/2} Z^{7/3} \alpha^{-3/2}
\]

finishing the result.
Of course, Lieb–Thirring faced the same problem and found a general solution that gives the inequality we need very quickly. They showed

\[ \sum \lambda_j (-\alpha \Delta + V) \leq c \alpha^{-3/2} \int |V(x)|^{5/2} dx \]

for any \( V \) and in our case \( \int |V(x; R)|^{5/2} dx = c R^{1/2} \) so they give \( |e_N| \leq c Z^{5/2} \alpha^{-3/2} R^{1/2} \).
We used a simple argument. For the truncated Coulomb to beat the central $\ell(\ell + 1)$ barrier, we know that only $\ell$’s below $L = O(Zr/\alpha)^{1/2} + 1$ entered. For allowed $\ell$’s, we used the full Coulomb and we got the bound we needed.