

A NUMBER–THEORETIC ESTIMATE FOR THE THOMAS–FERMI DENSITY.

Antonio Córdoba

Departamento de Matemáticas, Universidad Autónoma de Madrid
Cantoblanco, 28049 Madrid SPAIN

Charles L. Fefferman

*Department of Mathematics, Princeton University
Princeton NJ 08544 USA*

Luis A. Seco

*Department of Mathematics, University of Toronto
100 St. George St, Toronto ONTARIO M5S 1A1 CANADA*

Abstract

In this paper we obtain an estimate for the Thomas–Fermi density which plays a role in the analysis of the atomic energy asymptotics. Such estimate has obvious number–theoretic features related to the radial symmetry of a certain Schrödinger operator, and we use number–theoretic methods in our proof. From the technical viewpoint, we also simplify and improve some of the original estimates in the proof of the Dirac–Schwinger correction to the atomic energy asymptotics.

1 Introduction.

We denote the Thomas–Fermi potential for an atom of nuclear charge Z by $-V_{\text{TF}}^Z(|x|)$, and the Thomas–Fermi density by ρ_{TF}^Z , solutions to the Thomas–

Fermi equation

$$\begin{aligned}\Delta V_{\text{TF}}^Z &= 4\pi \rho_{\text{TF}}^Z \\ (V_{\text{TF}}^Z)^{3/2} &= 3\pi^2 \rho_{\text{TF}}^Z.\end{aligned}$$

In this paper we will be concerned with the density function defined by

$$\rho^{\text{NT}}(x) = |x|^{-2} \sum_{\ell=1}^{\ell_{\max}} (2\ell+1) \frac{\left(V_{\text{TF}}^Z(|x|) - \frac{\ell(\ell+1)}{|x|^2}\right)_+^{-1/2}}{\int_0^\infty \left(V_{\text{TF}}^Z(r) - \frac{\ell(\ell+1)}{r^2}\right)_+^{-1/2} dr} \cdot \mu(\phi_\ell), \quad x \in \mathbb{R}^3,$$

where $\mu(t) = t - [t + \frac{1}{2}]$, ($[s]$ denotes the greatest integer $\leq s$), and

$$\phi_\ell = \frac{1}{\pi} \int \left(V_{\text{TF}}^Z(r) - \frac{\ell(\ell+1)}{r^2}\right)_+^{1/2} dr.$$

Here, and throughout this article, we set

$$(x)_+^{-1/2} = \begin{cases} x^{-1/2} & \text{if } x > 0 \\ 0 & \text{if } x \leq 0. \end{cases}$$

Finally, ℓ_{\max} is the greatest integer such that $V_{\text{TF}}^Z(r) - \ell(\ell+1)/r^2$ is positive somewhere.

The main result of this paper is the estimate

$$\|\rho^{\text{NT}}\|_{\text{Coulomb}}^2 = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho^{\text{NT}}(x) \rho^{\text{NT}}(y)}{|x-y|} dx dy \leq C Z^\gamma, \quad \gamma < \frac{3}{2}. \quad (1.1)$$

Here, the Coulomb norm denotes

$$\|f\|_{\text{Coulomb}} = \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{f(x) f(y)}{|x-y|} dx dy.$$

If one removes the oscillating term $\mu(\phi_\ell)$ in the definition of ρ^{NT} , it is easy to see that (1.1) above fails: it would hold with $\gamma = \frac{5}{3}$ and this cannot be

improved. For ρ^{NT} however, it was proved in [FS6] that (1.1) holds for γ slightly smaller than $\frac{5}{3}$. The problem here lies in obtaining (1.1) for $\gamma < \frac{3}{2}$.

The relevance of (1.1) in atomic physics is as follows: denote the atomic ground state energy by $E(Z)$. It is conjectured (see [Fef]) that E admits the large- Z asymptotic expansion given by

$$E(Z) = -c_{\text{TF}} Z^{7/3} + \frac{1}{4} Z^2 + c_{\text{DS}} Z^{5/3} + \Psi(Z) + \text{error terms}, \quad (1.2)$$

where Ψ above is a certain oscillating function of size comparable to $Z^{3/2}$, which displays similar number theoretic features to our ρ^{NT} above. This conjecture follows naturally from the proof of the $Z^{5/3}$ -term given in [FS 1 – 8]; Ψ was analyzed in [CFS1] and [CFS2], where in particular it was also shown that Ψ contains classical mechanical features reminiscent of the Feynmann path integral formulation of quantum mechanics. We also refer the reader to [E], [ES1] and [ES2] for a physical discussion of oscillatory corrections to atomic energies.

The first three terms above are known rigorously (see [LS] for the first, [Hug] and [SW 1 – 3] for the second, and [FS 1 – 8] for the third; see also [IS] for the molecular case); their physical derivation dates back to [T] and [Fer], [Sco], [D] and [Sch] respectively. What remains to be done to establish the asymptotic formula (1.2) is to prove that all error terms are of size Z^γ with $\gamma < \frac{3}{2}$. It is here that the left hand side of (1.1) comes in, as one of those error terms. Moreover, (1.1) has the special feature that its nature is essentially number-theoretic, as opposed to the other error terms which are purely analytical and have to do with more or less accurate approximations to eigenvalues and eigenfunctions of certain Schrödinger operators, and with the analysis of electronic correlations.

Estimates such as (1.1) enter into the study of radially symmetric 3-dimensional Schrödinger operators as they quantify non-degeneracies among the different angular momentum channels. These non-degeneracies are related to the measure of closed trajectories of the corresponding classical Hamiltonian flow.

The number theoretic nature of estimate (1.1) is easily seen as follows: consider the related sum given by

$$\sum_{\ell=1}^{\ell_{\max}} \mu(\phi_{\ell}), \tag{1.3}$$

which is essentially just $\int \rho^{N^T}$. If we think of ϕ_{ℓ} as a curve parameterized by $\ell \in \mathbb{R}$ which encloses a domain $D \subset \mathbb{R}^2$, (1.3) corresponds to the error $N - E$ in estimating the number N of lattice points of \mathbb{Z}^2 inside D , by the volume E of D . If ϕ_{ℓ} were a circle, this would correspond to the circle problem, closely related to the number of representations of an integer as a sum of two squares: the radius R of the circle plays the role of our number ℓ_{\max} above. If ϕ_{ℓ} were a hyperbola, it would correspond to the divisor problem, equivalent to estimating the average of the number of divisors of large integers. Very powerful techniques have been developed for these problems (see, for instance, [CI], [Hux], [IM], [GK]) but an optimal answer, expected to be of the form (surface length) $^{\frac{1}{2}+\varepsilon}$, is yet unknown.

This partial number-theoretic knowledge has the following effect on our estimates: the trivial estimate for (1.3) of the form $C \ell_{\max}$ corresponds to $|N - E| \leq C R$ for the circle problem (a trivial geometric fact) and would give us (1.1) with $\gamma = \frac{5}{3}$. This would be far from satisfactory, since it allows the error terms in (1.2) to grow as large as the Dirac-Schwinger term. Estimate (1.1) with $\gamma < \frac{5}{3}$, (one of the results obtained in [FS6]) plays the role of bounds for the circle problem of the type R^{α} , with $\alpha < 1$. This is enough for the proof of the $Z^{5/3}$ -term in (1.2), but if one wants to single out Ψ in (1.2) as the next asymptotic term, one needs (1.1) with $\gamma < \frac{3}{2}$, which raises the question as to whether our current ability to analyze the circle problem and its analogues is enough for (1.1) with $\gamma < \frac{3}{2}$. The best estimate possible, yet unknown, for the circle problem, $R^{1/2+\varepsilon}$, intuitively corresponds to (1.1) with $\gamma = \frac{4}{3} + \varepsilon$, which -luckily- is more than we need. The fact that the standard techniques are enough to obtain (1.1) with $\gamma < \frac{3}{2}$, is therefore a fortunate fact.

2 Background material.

The Thomas–Fermi potential $-V_{\text{TF}}^Z$ satisfies the perfect scaling condition

$$V_{\text{TF}}^Z(r) = Z^{4/3} V\left(Z^{1/3} r\right),$$

for a universal function $V(r) > 0$. We also have

$$V(r) = \frac{y(a \cdot r)}{r}, \quad a = \left(\frac{3\pi}{2}\right)^{2/3}$$

where y is the Thomas–Fermi function, solution of the Thomas–Fermi equation

$$\left. \begin{aligned} y''(r) &= \frac{y^{3/2}(r)}{r^{1/2}} \\ y(0) &= 1 \\ \lim_{r \rightarrow \infty} y(r) &= 0. \end{aligned} \right\} \quad (2.1)$$

The constant a will be omitted in what follows.

Certain features of the Thomas–Fermi potential are most easily understood through the function $u(x) = x y(x)$. It has as main properties:

1. $u(x) = x + \mathcal{O}(x)$ as $x \rightarrow 0$;
2. Around infinity, $u(x) = 144 x^{-2} + \mathcal{O}(x^{-2-\alpha})$, with $\alpha = \frac{\sqrt{73}-7}{2}$, and $u^{(n)}(x) \sim c_n x^{-2-n}$.
3. u reaches a single maximum Ω_c^2 at the point r_c , and the equation $u(x) = \Omega^2$ has exactly two solutions $r_1(\Omega) < r_2(\Omega)$ for $\Omega \in (0, \Omega_c)$. In particular, $\ell_{\max} \sim Z^{1/3} \Omega_c$.

We refer the reader to [L1] for an excellent account of Thomas–Fermi theory, to [Hi] for basic details on the Thomas–Fermi function, and to [Hug], [SW2] and [FS6] for many of the other properties needed for atoms.

The only number–theoretic ingredient in our proof is the following estimate well–known to number–theorists:

Lemma (Number–Theory Lemma): *Suppose that $\phi(t)$ and $f(t)$ are defined on an interval $[0, S]$ ($S > 10$), and satisfy the estimates*

$$|f(t)| \leq C, \quad \text{Var}_{[0, S]} f \leq C, \quad b M^{-1} \leq \phi''(t) \leq C M^{-1}, \quad M \geq S.$$

Let μ be a periodic function of period 1, having average 0 and total variation on $[0, 1]$ bounded by C . Then, we have the estimate

$$\left| \sum_{0 \leq k \leq S} f(k) \mu(\phi(k)) \right| \leq \frac{C'}{b} M^{2/3} \log M,$$

where C' only depends on C above.

PROOF: Proofs of different versions of this go back to Hardy, Van der Corput, Vinogradov and others. A proof of this exact statement for $f \equiv 1$ can be found in [FS5], from which the case for f as above follows by summation by parts. \mathcal{Q}^D

3 Proof of the Theorem.

Consider the following norm acting on functions defined on the positive real line

$$\|\rho\|^2 = \int_0^\infty |\rho(R)|^2 \frac{dR}{R^2}.$$

In this way, since ρ^{NT} is a radial function, by Newton's theorem we have that

$$\|\rho^{\text{NT}}\|_{\text{Coulomb}} = \left\| \int_{|x| \leq R} \rho^{\text{NT}}(x) dx \right\|. \quad (3.1)$$

This identity, well known in quantum mechanics, can easily be seen as follows: for any radial function $f(|x|)$, the harmonicity of $1/|x|$ in $\mathbb{R}^3 - \{0\}$ implies

$$\begin{aligned} \|f(|\cdot|)\|_{\text{Coulomb}}^2 &= 2 \int_0^\infty \int_0^r f(r) f(s) \int_{|x|=r} \int_{|y|=s} \frac{1}{|x-y|} d\sigma(y) d\sigma(x) ds dr \\ &= 8 \pi \int_0^\infty \int_0^r f(r) f(s) \int_{|x|=r} \frac{s^2}{|x|} d\sigma(x) ds dr \\ &= 16 \pi^2 \int_0^\infty 2 r^2 f(r) \int_0^r f(s) s^2 ds \frac{dr}{r}. \end{aligned}$$

The identity in (3.1) then follows by integration by parts, since the integrand in the dr/r integral above equals $(d/dr)(\int_0^r f(s)s^2 ds)^2$.

Next, we use the perfect scaling of the Thomas–Fermi potential to rewrite ρ^{NT} as follows:

Set

$$u(x) = x y(x), \quad \Omega_\ell^2 = Z^{-2/3} \ell(\ell + 1), \quad \ell(\Omega) = -\frac{1}{2} + \frac{1}{2} \sqrt{1 + 4 \Omega^2 Z^{2/3}}.$$

Then,

$$\|\rho^{\text{NT}}\|_{\text{Coulomb}}^2 = Z^{1/3} \int_0^\infty \left| \sum_\ell (2\ell + 1) \mu(\phi_\ell) \cdot \frac{\int_0^R (u(x) - \Omega_\ell^2)_+^{-1/2} x dx}{\int_0^\infty (u(x) - \Omega_\ell^2)_+^{-1/2} x dx} \right|^2 \frac{dR}{R^2}.$$

Accordingly, we define

$$\begin{aligned} A(\Omega, R) &= \int_0^R (u(x) - \Omega^2)_+^{-1/2} x dx, & P(\Omega) &= \int_0^\infty (u(x) - \Omega^2)_+^{-1/2} x dx, \\ F(\Omega, R) &= \sqrt{Z^{-2/3} + 4 \Omega^2} \cdot \frac{A(\Omega, R)}{P(\Omega)}, & \phi(\Omega) &= \frac{1}{\pi} \int (u(x) - \Omega^2)_+^{1/2} \frac{dx}{x}, \end{aligned}$$

to obtain

$$\begin{aligned} \|\rho^{\text{NT}}\|_{\text{Coulomb}}^2 &= Z \int_0^\infty \left| \sum_\ell F(\Omega_\ell, R) \cdot \mu\left(Z^{1/3} \phi(\Omega_\ell)\right) \right|^2 \frac{dR}{R^2} \\ &= Z \|\tilde{\rho}^{\text{NT}}\|^2, \end{aligned} \tag{3.2}$$

where

$$\tilde{\rho}^{\text{NT}}(R) = \sum_{\ell=1}^{\ell_{\max}} F(\Omega_\ell, R) \cdot \mu\left(Z^{1/3} \phi(\Omega_\ell)\right).$$

At this point we will loose track of constants, and we adopt the convention that C and C' denote irrelevant large constants, c , c' denote irrelevant small constants, and C_i and c_i denote carefully chosen large and small constants, respectively.

Lemma 3.1: *Given $\Omega_1 < \Omega_2 < \Omega_c$ and $R > 0$, we have*

$$\text{Var}_{\Omega \in [\Omega_1, \Omega_2]} A(\Omega, R) \leq 2 \sup_{\Omega_1 \leq \Omega \leq \Omega_2} P(\Omega) + C \Omega_1^{-2}, \quad \text{all } R > 0,$$

where C is universal, independent of the Ω_i and R .

PROOF: We change variables in the integral as follows: Consider the increasing function

$$t(r) = \begin{cases} -(\Omega_c^2 - u(r))^{1/2} & \text{if } r \leq r_c, \\ (\Omega_c^2 - u(r))^{1/2} & \text{if } r \geq r_c, \end{cases}$$

which satisfies

$$\lim_{r \rightarrow 0} t(r) = -\Omega_c, \quad \lim_{r \rightarrow \infty} t(r) = \Omega_c,$$

and its inverse $r(t)$, which is also increasing and satisfies

$$\lim_{t \searrow -\Omega_c} r(t) = 0, \quad \lim_{t \nearrow \Omega_c} r(t) = \infty.$$

Set $D(\Omega) = \sqrt{\Omega_c^2 - \Omega^2}$. We then write

$$A(\Omega, R) = \int_{-D(\Omega)}^{t(R)} (D^2(\Omega) - t^2)_+^{-1/2} w(t) dt, \quad (w(t) = r(t) r'(t) > 0) \quad (3.3)$$

$$= \int_{-1}^{t(R)/D} (1 - t^2)_+^{-1/2} w(t D) dt. \quad (3.4)$$

As we prepare to obtain regularity properties of $w(t)$, note that, if ε is small, $\Omega_c - t(1/\varepsilon) \leq C u(1/\varepsilon) \leq C \varepsilon^2$, which implies $\Omega_c - \varepsilon^2 \leq t(C'/\varepsilon)$, which in turn implies

$$r(\Omega_c - \varepsilon) \leq C' \varepsilon^{-1/2}, \quad \varepsilon \text{ small enough.} \quad (3.5)$$

When t is close to Ω_c , we use $r'(t) = -2t/u'(r(t))$ to obtain

$$|w'(t)| = \left| \frac{-2r(t)}{u'(r(t))} + \frac{4t^2}{\{u'(r(t))\}^2} + \frac{2tr(t)r'(t)u''(r(t))}{\{u'(r(t))\}^2} \right| \leq C r^6(t),$$

$t > (1 - c_1) \Omega_c.$

Therefore, since $w'(t)$ is clearly bounded for $t < (1 - c_1)\Omega_c$, (3.5) yields

$$|w'(\Omega_c - \varepsilon)| \leq C \varepsilon^{-3}, \quad \varepsilon \in (0, 2\Omega_c). \quad (3.6)$$

Next, in order to compute the total variation of A , since D is a decreasing function of Ω , we may just as well consider A is a function of D , which will not change the total variation of A . Thus, we differentiate (3.4) with respect to D to obtain

$$\begin{aligned} & \frac{\partial A(\Omega, R)}{\partial D} \\ &= - \left(1 - \frac{t(R)^2}{D^2}\right)_+^{-1/2} w(t(R)) \frac{t(R)}{D^2} + \int_{-1}^{t(R)/D} (1 - t^2)_+^{-1/2} w'(tD) t dt. \end{aligned}$$

The first term above is negative when $R > r_c$, and positive when $R < r_c$, by (3.3); in other words, as a function of D , it does not change sign. Therefore,

$$\left| \frac{\partial A(\Omega, R)}{\partial D} \right| \leq \text{sign}(r_c - R) \frac{\partial A(\Omega, R)}{\partial D} + 2 \int_{-1}^{t(R)/D} (1 - t^2)_+^{-1/2} |w'(tD) t| dt,$$

which yields

$$\begin{aligned} & \int_{D(\Omega_2)}^{D(\Omega_1)} \left| \frac{\partial A(\Omega, R)}{\partial D} \right| dD \\ & \leq |A(\Omega_1, R) - A(\Omega_2, R)| + 2 \int_{D(\Omega_2)}^{D(\Omega_1)} \int_{-1}^1 (1 - t^2)^{-1/2} |w'(tD) t| dt dD. \end{aligned}$$

Thus, it remains only to analyze the last double integral above. In order to do that, observe that tD , over the domain of integration, satisfies

$$\Omega_c - tD \geq \Omega_c - (\Omega_c^2 - \Omega^2)^{1/2} \geq c\Omega^2 = c(\Omega_c^2 - D^2) \geq c'(\Omega_c - D).$$

By (3.6) we then conclude that $w'(tD) \leq C/(\Omega_c - D)^3$. Hence,

$$\begin{aligned} & \int_{D(\Omega_2)}^{D(\Omega_1)} \int_{-1}^1 (1 - t^2)^{-1/2} |w'(tD) t| dt dD \\ & \leq C \int_{D(\Omega_2)}^{D(\Omega_1)} \int_{-1}^1 (1 - t^2)^{-1/2} \frac{|t|}{(\Omega_c - D)^3} dt dD \\ & \leq C (\Omega_c - D)^{-2} \Big|_{D(\Omega_2)}^{D(\Omega_1)} \\ & \leq C \Omega_1^{-2}, \end{aligned}$$

as needed. \mathcal{Q}^D

Lemma 3.2: *Let $Z^{-1/3} \leq \Omega_1 \leq \Omega_2 \leq 10\Omega_1$. Then,*

$$|F(\Omega, R)| \leq C \Omega_2, \quad \text{Var}_{\Omega \in [\Omega_1, \Omega_2]} F(\Omega, R) \leq C \Omega_2,$$

for a universal constant C , independent of Z , R and the Ω_i .

PROOF: We use the product formula

$$\text{Var}(f \cdot g) \leq \text{Var} f \cdot \sup g + \text{Var} g \cdot \sup f.$$

For P , we use a result obtained in [CFS2], which says that $P(\Omega) \geq c\Omega^{-3}$ and $P^{(k)}(\Omega) \leq C_k \Omega^{-3-k}$ for all $k \geq 0$.

For $A(\Omega, R)$ we use Lemma 3.1, together with the obvious fact $A(\Omega, R) \leq P(\Omega)$.

The lemma then follows from the product formula with the equally obvious fact:

$$\sqrt{Z^{-2/3} + 4\Omega^2} \leq 8\Omega, \quad \left| \frac{d}{d\Omega} \sqrt{Z^{-2/3} + 4\Omega^2} \right| \leq 10. \quad \mathbb{Q}^D$$

Once the regularity for the amplitude function F has been settled, we would like to go ahead and use the Number Theory Lemma. However, ϕ'' does not satisfy the right regularity bounds: it was shown in [CFS2] that

$$c\Omega^{\alpha-1} \leq \phi''(\Omega) \leq C\Omega^{\alpha-1}, \quad |\phi'(\Omega)| \leq C, \quad \alpha = \frac{\sqrt{73}-7}{2}. \quad (3.7)$$

In particular, if we use the number-theory lemma directly, the discrepancy between the size of ϕ'' near 0 and near Ω_c will cause error bounds to blow up. Therefore, we will need an extra localization argument.

Theorem 3.3: *We have*

$$\|\rho^{\text{NT}}\|_{\text{Coulomb}}^2 \leq C Z^{13/9} \log^2 Z.$$

PROOF: By (3.2), it will be enough to estimate $\|\tilde{\rho}^{\text{NT}}\|$.

Set $L = C_1 Z^{1/9}$. Construct a partition of $[L, \ell_{\max}]$ given by $\{U_\nu\}$ for $\nu = 0, 1, \dots, \nu_{\max}$, such that

$$U_\nu = [a_\nu, b_\nu], \quad a_\nu = 2^{-\nu-1} \cdot \ell_{\max}, \quad b_\nu = 2^{-\nu} \cdot \ell_{\max},$$

and break up $\tilde{\rho}^{\text{NT}}$ into

$$\tilde{\rho}^{\text{NT}}(R) = \tilde{\rho}_{\text{TRIVIAL}}(R) + \sum_{\nu} \rho_\nu(R), \quad (3.8)$$

with

$$\begin{aligned} \tilde{\rho}_{\text{TRIVIAL}}(R) &= \sum_{1 \leq \ell < L} F(\Omega_\ell, R) \cdot \mu\left(Z^{1/3} \phi(\Omega_\ell)\right), \\ \rho_\nu(R) &= \sum_{a_\nu \leq \ell < b_\nu} F(\Omega_\ell, R) \cdot \mu\left(Z^{1/3} \phi(\Omega_\ell)\right). \end{aligned}$$

We first estimate $\tilde{\rho}_{\text{TRIVIAL}}$ trivially –of course– as follows: each term in the sum is 0 when $R < r_1(\Omega_\ell)$. Therefore, the sum is taken over ℓ such that $\ell(\ell+1) \leq u(R) Z^{2/3}$, and hence contains at most $\min\left\{L, Z^{1/3} R^{1/2}\right\}$ terms, each of which is trivially bounded by $C Z^{-1/3} L$. Moreover, $R \geq r_1(\Omega_1) \geq Z^{-2/3}$. Therefore,

$$\begin{aligned} \|\tilde{\rho}_{\text{TRIVIAL}}\|^2 &\leq C \int_{Z^{-2/3}}^{L^2 Z^{-2/3}} L^2 \frac{dR}{R} + C \int_{L^2 Z^{-2/3}}^{\infty} L^4 Z^{-2/3} \frac{dR}{R^2} \\ &\leq C Z^{2/9} \log Z. \end{aligned} \quad (3.9)$$

The rest of the ρ_ν will be estimated using our elementary number theory. In preparation to use the Number–Theory Lemma, note that the total variation of $F(\Omega_\ell, R)$ as a function of $\ell \in U_\nu$ is the same as the total variation of $F(\Omega, R)$ as a function of $\Omega \in [\Omega_{a_\nu}, \Omega_{b_\nu}]$, since we obtain one from the other by composition with a monotone function. Since, for $\Omega \in [\Omega_{a_\nu}, \Omega_{b_\nu}]$ we have $\Omega \sim \Omega_{a_\nu} \sim \Omega_{b_\nu}$, Lemma 3.2 implies

$$\text{Var}_{\Omega \in [\Omega_{a_\nu}, \Omega_{b_\nu}]} F(\Omega, R) \leq C \Omega_{a_\nu}.$$

We now turn our attention to ϕ_ℓ :

$$\frac{d^2\phi(\Omega_\ell)}{d\ell^2} = \frac{(\ell + \frac{1}{2})^2}{\ell(\ell + 1)}\phi''(\Omega_\ell) Z^{-2/3} - \frac{\phi'(\Omega_\ell)}{4(\ell(\ell + 1))^{3/2}} Z^{-1/3}.$$

If $\ell \geq C_1 Z^{1/9}$, the last term above is bounded by $Z^{-2/3}$. Moreover, if we take C_1 large enough, since $1 \leq (\ell^2 + \ell + \frac{1}{4})/(\ell^2 + \ell) \leq 2$, by (3.7) we obtain

$$c\Omega_\ell^{-1+\alpha} Z^{-2/3} \leq \frac{d^2\phi(\Omega_\ell)}{d\ell^2} \leq C\Omega_\ell^{-1+\alpha} Z^{-2/3}.$$

Since any $\Omega \in [\Omega_{a_\nu}, \Omega_{b_\nu}]$ is comparable to Ω_{a_ν} , we use the Number–Theory Lemma with

$$S = b_\nu - a_\nu, \quad M = b_\nu \cdot \left(\frac{\Omega_{b_\nu}}{\Omega_c}\right)^{-\alpha}, \quad f(\ell) = \Omega_{a_\nu}^{-1} \cdot F(\Omega_\ell, R),$$

to conclude that

$$|\rho_\nu(R)| \leq C\Omega_{a_\nu}^{\frac{5}{3}-\frac{2\alpha}{3}} \cdot Z^{2/9} \log Z. \quad (3.10)$$

Note that if $r_1(\Omega_\ell) \geq R$, then $F(\Omega_\ell, R) = 0$; therefore $\rho_\nu(R) = 0$ when $R < \frac{1}{4}\Omega_{a_\nu}^2$ and we only need to use (3.10) when $R \geq \frac{1}{4}\Omega_{a_\nu}^2$. In this way we obtain

$$\begin{aligned} \|\rho_\nu\|^2 &\leq C Z^{4/9} \log^2 Z \cdot \Omega_{a_\nu}^{\frac{10}{3}-\frac{4\alpha}{3}} \int_{\frac{1}{4}\Omega_{a_\nu}^2}^{\infty} \frac{dR}{R^2} \\ &\leq C Z^{4/9} \log^2 Z \cdot \Omega_{a_\nu}^{\frac{4}{3}(1-\alpha)}. \end{aligned} \quad (3.11)$$

Hence, putting (3.11) and (3.9) into (3.8) we conclude

$$\begin{aligned} \|\tilde{\rho}^{\text{NT}}\| &\leq C Z^{1/9} (\log Z)^{1/2} + C \sum_{\nu}^{\nu_{\max}} 2^{-2\nu(1-\alpha)/3} Z^{2/9} \log Z \\ &\leq C Z^{2/9} \log Z. \end{aligned}$$

Then, (3.2) finishes the proof. \mathcal{Q}^D

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