THE DENSITY IN A THREE-DIMENSIONAL RADIAL POTENTIAL

by

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Introduction

Let $H = -\Delta + V$ be a Schrödinger operator on $\mathbb{R}^n$. The *density* associated to H is defined as

$$(1) \qquad \rho(x) = \sum_{E_k \le 0} |\varphi_k(x)|^2 ,$$

where E_k, φ_k are the eigenvalues and normalized eigenfunctions of H. A standard approximation to ρ is the *semiclassical density*, given by

$$(2) \qquad \rho_{sc}(x) = c_n \big(-V(x)\big)_+^{n/2} \quad (x \in \mathbb{R}^n) ,$$

where $c_n > 0$ depends only on the dimension n, and $t_+^s \equiv \begin{cases} t^s & \text{if } t > 0 \\ 0 & \text{otherwise} \end{cases}$.

The purpose of this paper is to estimate $\rho - \rho_{sc}$ for a particular potential V_{TF} on $\mathbb{R}^3$, that arises in the study of atoms. Specifically, $V_{TF}(x)$ is the Thomas-Fermi potential for atomic number Z; we will describe V_{TF} below.

In [FS1], we announced the proof of an asymptotic formula for the ground-state energy of a non-relativistic atom. A crucial step in the proof of that formula is the estimate

$$(3) \qquad \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \big(\rho(x) - \rho_{sc}(x)\big)\big(\rho(y) - \rho_{sc}(y)\big) \frac{dx\, dy}{|x-y|} \le C Z^{5/3-a} \ (a > 0) ,$$

where ρ and ρ_{sc} arise from V_{TF} for large Z. The main result of this paper is that (3) holds, modulo an assumption which will be proven in our later papers [FS6,7]. The complete proof of the theorem in [FS1] is given by this paper, together with [FS2...7].

The potential V_{TF} for an atom is spherically symmetric. Hence, it is natural to prove (3) by separation of variables. Recall that the density ρ associated to a radial potential $V(|x|)$ on $\mathbb{R}^3$ is given by

$$(4) \qquad \rho(x) = \frac{1}{4\pi |x|^2} \sum_{\ell \ge 0} (2\ell + 1) \rho_\ell(|x|) ,$$

where $\rho_\ell(r)$ is the density associated to $-\frac{d^2}{dr^2} + V_\ell(r)$ on $(0,\infty)$, with

$$V_\ell(r) = \frac{\ell(\ell+1)}{r^2} + V(r) \ . \tag{5}$$

The results of our earlier paper [FS4] allow us to compute $\rho_\ell(r)$ modulo errors whose total contribution to (4) will not affect (3).

In fact, for suitable one-dimensional potentials W on $(0,\infty)$, we proved in [FS4] that the density is well-approximated by

$$\tilde{\rho}_{sc}(x) = \frac{1}{\pi}\big(-W(x)\big)_+^{1/2} - \frac{\big(-W(x)\big)_+^{-1/2}}{\mathcal{N}}\chi_-(\phi) \ , \quad \text{where} \tag{6}$$

$$\mathcal{N} = \int_0^\infty \big(-W(x)\big)_+^{-1/2} dx \ , \quad \phi = \frac{1}{\pi}\int_0^\infty \big(-W(x)\big)_+^{1/2} dx - \frac{1}{2} \ , \quad \text{and} \tag{7}$$

$$\chi_-(t) = t - k - \frac{1}{2} \ , \quad \text{with } k = \ (\text{greatest integer } \le t) \ . \tag{8}$$

On the right in (6), the first term is the usual semi-classical approximation, while the second term is a small correction.

Taking $W = V_\ell$ and putting (6) into (4), we see that

$$\begin{aligned}\rho(x) \approx \frac{1}{4\pi|x|^2} \sum_{\ell\ge 0} (2\ell+1)\cdot\frac{1}{\pi}\big(-V_\ell(|x|)\big)_+^{1/2} \\ - \frac{1}{4\pi|x|^2}\sum_{\ell\ge 0}\frac{(2\ell+1)}{\mathcal{N}_\ell}\chi_-(\phi_\ell)\cdot\big(-V_\ell(|x|)\big)_+^{-1/2} \ ,\end{aligned} \tag{9}$$

with

$$\mathcal{N}_\ell = \int_0^\infty \big(-V_\ell(r)\big)_+^{-1/2} dr \ , \quad \phi_\ell = \frac{1}{\pi}\int_0^\infty \big(-V_\ell(r)\big)_+^{1/2} dr - \frac{1}{2} \ . \tag{10}$$

The first term on the right in (9) is a Riemann sum, which closely approximates the integral

$$\int_0^\infty \frac{(2\lambda+1)}{4\pi|x|^2}\cdot\frac{1}{\pi}\left(-\frac{\lambda(\lambda+1)}{|x|^2} - V(x)\right)_+^{1/2} d\lambda \ .$$

This integral is equal to the semiclassical density (2). Thus, (9) yields

$$\rho(x) - \rho_{sc}(x) \approx \rho_{NT}(x)\ , \quad \text{with} \tag{11}$$

$$\rho_{NT}(x) = -\frac{1}{4\pi|x|^2} \sum_{\ell \geq 0} \frac{(2\ell+1)}{\mathcal{N}_\ell} \chi_-(\phi_\ell) \cdot \left(-V_\ell(|x|)\right)_+^{-1/2} . \tag{12}$$

So the basic estimate (3) amounts to saying that

$$\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \rho_{NT}(x) \rho_{NT}(y)\ \frac{dx dy}{|x-y|} \leq C\, Z^{\frac{5}{3}-a}\ (a > 0)\ . \tag{13}$$

when V is the Thomas-Fermi potential for atomic number Z.

Let us see what is needed to prove (13). A glance at the definition (8) shows that $|\chi_-(t)| \leq \frac{1}{2}$ for any t. Hence we have the trivial estimate

$$|\rho_{NT}(x)| \leq \rho^+(x) \equiv \frac{1}{4\pi|x|^2} \sum_{\ell \geq 0} \frac{(2\ell+1)}{\mathcal{N}_\ell} \left(-V_\ell(|x|)\right)_+^{-1/2} .$$

One computes easily that $\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \rho^+(x) \rho^+(y) \frac{dxdy}{|x-y|}$ has the order of magnitude $Z^{5/3}$. Thus, (13) means that significant cancellation occurs in the sum (12). Such cancellation occurs if the ϕ_ℓ are equidistributed modulo 1, since $\chi_-(t)$ has period 1 and mean zero. In this paper, we make assumptions on the equidistribution of the ϕ_ℓ modulo 1. These assumptions will be proven in [FS6,7].

To state our assumptions on the ϕ_ℓ, we introduce $\ell_{\max}$, the largest angular momentum for which $V_\ell(r)$ is negative somewhere. (The order of magnitude of $\ell_{\max}$ is $Z^{1/3}$.) Our assumptions on the ϕ_ℓ are as follows.

(A) There are at most $CZ^{-\frac{1}{3}-2a}$ integers $\ell \leq \ell_{\max}$ for which
$|\phi_\ell - (\text{nearest integer})| \leq \ell^{-6/43}$.

(B) For $Z^{(10^{-9})} \leq \ell_1 < \ell_2 \leq \ell_{\max}$, with $\ell_2 - \ell_1 > \ell_{\max}^{1-10a}$, we have
$\left| \sum_{\ell_1 \leq \ell \leq \ell_2} \frac{(2\ell+1)}{\mathcal{N}_\ell} \chi_-(\phi_\ell) \right| \leq C\, Z^{-\frac{2}{3}a} \sum_{\ell_1 \leq \ell \leq \ell_2} \frac{(2\ell+1)}{\mathcal{N}_\ell}$.

Here, $0 \le a < 1/43$. The indices here are rather arbitrary, but at least (A) and (B) express the equidistribution of the ϕ_ℓ modulo 1.

The main result of this paper is that (A) and (B) imply the estimate

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \big(\rho(x)-\rho_{sc}(x)\big)\big(\rho(y)-\rho_{sc}(y)\big)\frac{dxdy}{|x-y|} \le C\, Z^{\frac{5}{3}-\ \frac{2}{3}a} \ .$$

In [FS6,7], we show that (A) and (B) hold for some positive a.

Although we forgo a serious discussion of (A) and (B) here, we should point out that they are intimately connected with the scarcity of periodic, zero energy orbits for the Thomas-Fermi potential V_{TF}. To illustrate this point, consider the harmonic oscillator $V_1(x) = A|x|^2 - B$ or the hydrogenic potential $V_2(x) = E - \frac{Z}{|x|}$ on $\mathbb{R}^3$. These potentials scale like the Thomas-Fermi potential if we take $A \sim Z^2$, $B \sim Z^{4/3}$, $E \sim Z^{4/3}$. Of course, V_1 and V_2 are classical examples of potentials with many periodic orbits. One checks easily that (3), (13) and (B) all fail for V_1 and V_2.

Next, we give a layman's explanation of the Thomas-Fermi potential. As a simplified model of an atom, we imagine a nucleus of charge Z fixed at the origin, and an electron cloud with particle density $\rho(x)$ on $\mathbb{R}^3$. Each electron in the cloud feels the attraction of the nucleus and the repulsion of the electron cloud. Therefore, each electron behaves as if it were governed by the Hamiltonian $H = -\Delta + V$, with

$$V(x) = -\frac{Z}{|x|} + \int_{\mathbb{R}^3}\frac{\rho(y)dy}{|x-y|} \ . \tag{14}$$

On the other hand, the density of electrons governed by the Hamiltonian H is given by (1). In the semiclassical approximation, therefore,

$$\rho(x) = (\mathrm{const})\big(-V(x)\big)^{3/2} \ . \tag{15}$$

The solution of equations (14), (15) is given by the *Thomas-Fermi density* $\rho_{TF}(x)$ and the *Thomas-Fermi potential* $V_{TF}(x)$. These functions are radially symmetric, and (14), (15) reduce to an ordinary differential equation. In fact, one finds that

$$V_{TF}(x) = cZ^{4/3} V_1(cZ^{1/3}|x|) \quad \text{for a constant } c\ , \text{ with} \tag{16}$$

$$V_1(t) = t^{-1} y(t)\ , \tag{17}$$

and $y(t)$ defined as the solution of the *Thomas-Fermi equation*

$$\frac{d^2}{dt^2}\, y(t) = t^{-1/2}\big(y(t)\big)^{3/2} \text{ on } (0,\infty)\ ;\quad y(0) = 1\ ,\quad y(\infty) = 0\ . \tag{18}$$

From (16)...(18), one can read off the basic properties of V_{TF}. For instance, the order of magnitude of V_{TF} is given by

$$-V_{TF}(x) \sim \min\left\{Z|x|^{-1}, |x|^{-4}\right\} \quad (x \in \mathbb{R}^3)\ . \tag{19}$$

A detailed discussion of Thomas-Fermi theory is given by Lieb [L].

We close this introduction by mentioning several open problems on the density (1). The first natural problem is to estimate $\rho - \rho_{sc}$ for the Thomas-Fermi potential of a molecule. The most we can hope for here is probably

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \big(\rho(x) - \rho_{sc}(x)\big)\big(\rho(y) - \rho_{sc}(y)\big)\frac{dxdy}{|x-y|} = o(Z^{5/3}) \tag{20}$$

in place of (3). The proof of (20) ought to involve wave-equation methods since it brings in the aperiodicity of the Hamiltonian flow.

The next problem concerns formula (11), whose precise meaning is as follows.

$$\rho(x) - \rho_{sc}(x) = \rho_{{}_{NT}}(x) + g(x)\ ,\quad \text{with} \tag{21}$$

$$\int\!\!\!\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{g(x)g(y)}{|x-y|} dxdy \le CZ^{5/3-\gamma} \quad (\gamma > 0)\ . \tag{22}$$

This is enough to accomplish the purpose of (11), namely the reduction of (3) to (13). However, we believe that (22) can be sharpened considerably, by taking γ

larger. If γ is large enough, then (21) and (22) identify ρ_{NT} as the leading correction to the semiclassical density for a given potential V.

We would like to understand the function ρ_{NT}. This brings in analytic number theory. For instance, the computation of $\int_{\mathbb{R}^3} \rho_{NT}(x)dx = \sum_{\ell \leq \ell_{\max}} (2\ell+1)\chi_-(\phi_\ell)$ seems very close to that of $\sum_{\ell \leq \ell_{\max}} \chi_-(\phi_\ell)$, which in turn is clearly equivalent to counting the lattice points in the plane domain $\{(\lambda, \xi) : 0 \leq \xi < \Phi(\lambda)\}$, with

$$\Phi(\lambda) = \frac{1}{\pi} \int_0^\infty \big(-\frac{\lambda(\lambda+1)}{r^2} - V_{TF}(r)\big)_+^{1/2} dr - \frac{1}{2} \ .$$

Our current understanding of lattice-point problems appears to be inadequate to answer basic questions about the size and fluctuations of ρ_{NT}.

Finally, we point out that if ρ_{NT} is indeed the leading correction to the semiclassical density, then we can write a corrected equation in place of (15). Combining that new equation with (14) and solving by perturbation theory, we hope to find the leading correction to the Thomas-Fermi density. This would suggest that the density of electrons in a non-relativistic atom has a number-theoretic character.

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Review of Earlier results

In this section, we recall the main results from our previous paper [FS4] on one-dimensional potentials.

A. The WKB Density Theorem in One Dimension

Set-Up: We are given positive numbers ε, K, N, $\hat{c}$; two intervals $I \subset I_{\mathrm{BVP}}$ (possibly unbounded); a point $x_0 \in I$; a potential $V(x)$ defined on I_{BVP}; and two positive functions $S(x)$, $B(x)$ defined on I. Our assumptions are as follows.

Assumptions Concerning $V(x)$, $S(x)$, $B(x)$ on I.

(Z0) If $x, y \in I$ and $|x - y| < cB(x)$, then $c < \frac{B(y)}{B(x)} < C$ and $c < \frac{S(y)}{S(x)} < C$.

(Z1) If $x \in I$ and $\alpha \geq 0$, then $\left|\left(\frac{d}{dx}\right)^{\alpha} V(x)\right| \leq C_\alpha S(x) B^{-\alpha}(x)$.

(Z2) The set $\{x \in I \mid V(x) < 0\}$ is a non-empty interval $(x_{\mathrm{left}}, x_{\mathrm{rt}})$, with $\mathrm{dist}\,(x_{\mathrm{left}}, \partial I) > cB(x_{\mathrm{left}})$ and $\mathrm{dist}\,(x_{\mathrm{rt}}, \partial I) > cB(x_{\mathrm{rt}})$.

(Z3) We have $V(x_0) < -cS(x_0)$, $V'(x_0) = 0$; and for $|x - x_0| \leq c_1 B(x_0)$ we have $V''(x) \geq cS(x_0) B^{-2}(x_0)$.

(Z4) For $x_{\mathrm{left}} \leq x \leq x_0 - c_1 B(x_0)$ we have $-V'(x) > cS(x)B^{-1}(x)$; and for $x_0 + c_1 B(x_0) \leq x \leq x_{\mathrm{rt}}$ we have $+V'(x) > cS(x)B^{-1}(x)$.

Define $\lambda(x) = S^{1/2}(x)B(x)$ for $x \in I$, and set

$$\Lambda = \left(\int_{x_{\mathrm{left}}}^{x_{\mathrm{rt}}} \frac{dx}{\lambda(x) B(x)} \right)^{-1} .$$

Assumptions Concerning $V(x)$ on all of I_{BVP}.

(Z5) We have $V(x) > 0$ for all $x \in I_{\mathrm{BVP}} \backslash [x_{\mathrm{left}}, x_{\mathrm{rt}}]$.

(Z6) For all $x \in I_{\mathrm{BVP}}$ with $x < x_{\mathrm{left}} - \Lambda^K B(x_{\mathrm{left}})$, we have $V(x) \geq \frac{1000}{|x - x_{\mathrm{left}}|^2}$; and for all $x \in I_{\mathrm{BVP}}$ with $x > x_{\mathrm{rt}} + \Lambda^K B(x_{\mathrm{rt}})$, we have $V(x) \geq \frac{1000}{|x - x_{\mathrm{rt}}|^2}$.

Polynomial Growth Assumptions on $S(x)$, $B(x)$, I.

(Z7) We have $\max_{x\in I} B(x) < \Lambda^K \min_{x \in I} B(x)$; $\max_{x \in I} S(x) < \Lambda^K \min_{x\in I} S(x)$; and $|I| < \Lambda^K \cdot \min_{x \in I} B(x)$.

Smallness of the Constant $\hat{c}$.

(Z8) The constant $\hat{c}$ is bounded above by a certain small, positive number determined by ε, K, N, c, C, c_1, C_α.

The WKB Hypothesis.

(Z9) Λ is bounded below by a certain large, positive number determined by ε, K, N, c, C, c_1, $\hat{c}$, C_α.

Let E_k and $u_k(x)$ be the eigenvalues and (normalized) eigenfunctions of $-\frac{d^2}{dx^2} + V(x)$ on I_{BVP}, with Dirichlet or Neumann boundary conditions. Then define the density $\rho(x)$ and its refined semiclassical approximation $\tilde{\rho}_{sc}(x)$ on I_{BVP} by setting:

$$\rho(x) = \sum_{E_k \le 0} |u_k(x)|^2 \quad (x \in I_{\mathrm{BVP}}) \ ;$$

$$\tilde{\rho}_{sc}(x) = \frac{1}{\pi}\big(-V(x)\big)_+^{1/2} - \frac{\big(-V(x)\big)_+^{-1/2}}{\int_{I_{\mathrm{BVP}}} \big(-V(y)\big)_+^{-1/2} dy} \chi_-\Big(\frac{1}{\pi}\int_{I_{\mathrm{BVP}}} \big(-V(y)\big)_+^{1/2} dy - \frac{1}{2}\Big) \quad (x \in I_{\mathrm{BVP}}) \ .$$

Recall that $t_+^a = t^a$ for $t > 0$, $t_+^a = 0$ for $t \le 0$, and that $\chi_-(t) = x - k - \frac{1}{2}$ for $k =$ (largest integer $\le x$).

For any $x \in \mathbb{R}$, define

$$H(x) = \int_{I_{\mathrm{BVP}} \cap (-\infty, x]} (\rho(\overline{x}) - \tilde{\rho}_{sc}(\overline{x})) d\overline{x} \ .$$

WKB Density Theorem. *Assume (Z0)... (Z9).*

Case I: Suppose $\min_{k \in \mathbb{Z}} \left| \int_{I_{\mathrm{BVP}}} \big(-V(y)\big)_+^{1/2} dy - \pi(k + 1/2) \right| > \overline{C}\Lambda^{-1}$. *Then*

(A) $$|H(x)| \le \Lambda^{-N} \quad \textit{for} \quad x \le x_{\mathrm{left}} - \hat{c}B(x_{\mathrm{left}}) \ .$$

(B) $$\Big(Av_{|x - \tilde{x}| < \hat{c}B(\tilde{x})} |H(x)|^2\Big)^{1/2} \le \Lambda^{-N} + C_* \Lambda^{\varepsilon - \frac{45}{43}} \int_{I_{\mathrm{BVP}} \cap (-\infty, \tilde{x} + \overline{C}\hat{c}B(\tilde{x})]} \big(-V(y)\big)_+^{1/2} dy$$
$$\textit{for} \quad x_{\mathrm{left}} - \hat{c}B(x_{\mathrm{left}}) \le \tilde{x} \le x_{\mathrm{rt}} + \hat{c}B(x_{\mathrm{rt}}) \ .$$

(C) $$|H(x)| \leq \Lambda^{-N} + C_* \Lambda^{\varepsilon - \frac{45}{43}} \int_{I_{\mathrm{BVP}}} \left(-V(y)\right)_+^{1/2} dy \quad \textit{for} \quad x \geq x_{\mathrm{rt}} + \hat{c} B(x_{\mathrm{rt}}) \ .$$

Case II: Suppose instead $\min_{k \in \mathbb{Z}} \left| \int_{I_{\mathrm{BVP}}} \left(-V(y)\right)_+^{1/2} dy - \pi(k+1/2) \right| \leq \overline{C} \Lambda^{-1}$*. Then*

(A) $$|H(x)| \leq \Lambda^{-N} \quad \textit{for} \quad x \leq x_{\mathrm{left}} - \hat{c} B(x_{\mathrm{left}}) \ .$$

(B) $$\left(Av_{|x - \tilde{x}| < \hat{c} B(\tilde{x})} |H(x)|^2 \right)^{1/2} \leq \Lambda^{-N} + C_* \Lambda^{-1} \int_{I_{\mathrm{BVP}} \cap (-\infty, \tilde{x} + \overline{C} \hat{c} B(\tilde{x})]} \left(-V(y)\right)_+^{1/2} dy$$
$$\textit{for} \quad x_{\mathrm{left}} - \hat{c} B(x_{\mathrm{left}}) \leq \tilde{x} \leq x_{\mathrm{rt}} + \hat{c} B(x_{\mathrm{rt}}) \ .$$

(C) $$|H(x)| \leq \Lambda^{-N} + C_* \Lambda^{-1} \int_{I_{\mathrm{BVP}}} \left(-V(y)\right)_+^{1/2} dy \quad \textit{for} \quad x \geq x_{\mathrm{rt}} + \hat{c} B(x_{\mathrm{rt}}) \ .$$

Here $\overline{C}$ *depends only on* ε, K, N, c, C, c_1, C_α*; and* C_* *depends only on* ε, K, N, c, C, c_1, $\hat{c}$, C_α.

Remarks. The exponent $\varepsilon - \frac{45}{43}$ in *Case I* is not important to us in this paper, and surely not optimal. Any exponent strictly less than -1 would serve our purpose.

B. The Density for Degenerate One-Dimensional Potentials I

In the next sections, we prove crude results on the density $\rho(x)$ in various degenerate cases in which the hypotheses in the preceding section break down. We begin by treating a potential $V(x)$ whose minimum $V(x_0)$ is negative but has relatively small absolute value.

Set-up. We are given positive numbers ε, K, N, S, B; a potential $V(x)$ defined on a (possibly unbounded) interval I_{BVP}; and a point $x_0 \in I_{\mathrm{BVP}}$. Our assumptions are as follows.

Hypotheses

(Z0*) $I = \{x \colon |x - x_0| < cB\} \subset I_{\mathrm{BVP}}$.

(Z1*) $\left|\left(\frac{d}{dx}\right)^\alpha V(x)\right| \le C_\alpha S B^{-\alpha}$ on I.

(Z2*) $V''(x) \ge c' S B^{-2}$ on I.

Set $\lambda = S^{1/2}B$, and make the following further assumptions.

(Z3*) $V'(x_0) = 0$ and $-\lambda^{-\frac{36}{43}} S \le V(x_0) < 0$.

(Z4*) For $x \in I_{\mathrm{BVP}} \backslash I$ we have $V(x) > 0$.

(Z5*) For $x \in I_{\mathrm{BVP}}$ with $|x - x_0| > \frac{1}{2}\lambda^K B$, we have $V(x) \ge \frac{1000}{|x-x_0|^2}$.

(Z6*) λ is bounded below by a certain large, positive number determined by ε, K, N, c, c', C_α.

Let E_k, $u_k(x)$ be the eigenvalues and (normalized) eigenfunctions for $-\frac{d^2}{dx^2} + V(x)$ on I_{BVP}, with Dirichlet or Neumann boundary conditions.

As in the previous section, define the density $\rho(x)$ and its refined semiclassical approximation $\tilde{\rho}_{sc}(x)$ on I_{BVP}, by the formulas

$$\rho(x) = \sum_{E_k \le 0} |u_k(x)|^2$$

$$\tilde{\rho}_{sc}(x) = \frac{1}{\pi}\big(-V(x)\big)_+^{1/2} - \frac{\big(V(x)\big)_+^{-1/2}}{\int_{I_{\mathrm{BVP}}}\big(-V(y)\big)_+^{-1/2} dy}\, \chi_-\Big(\frac{1}{\pi}\int_{I_{\mathrm{BVP}}}\big(-V(y)\big)_+^{1/2} dy - \frac{1}{2}\Big)$$

Then set

$$H(x) = \int_{I_{\mathrm{BVP}} \cap (-\infty, x]} \big(\rho(\overline{x}) - \tilde{\rho}_{sc}(\overline{x})\big)\, d\overline{x}\ .$$

First Degenerate Density Lemma. *Assume (Z0*)... (Z6*).*

CASE I: Suppose $\min_{k\in\mathbb{Z}}\left|\int_{I_{\mathrm{BVP}}}\big(-V(y)\big)_+^{1/2} dy - \pi(k+1/2)\right| \ge \overline{C}\lambda^{-1}$. *Then*

(A) $|H(x)| \le \lambda^{-N}$ *if* x *lies to the left of* I.

(B) $\big(Av_I |H|^2\big)^{1/2} \le C_* \lambda^{\varepsilon - 2/43}$.

(C) $|H(x)| \le C_* \lambda^{\varepsilon - 2/43}$ *if* x *lies to the right of* I.

CASE II: Suppose instead $\min_{k\in\mathbb{Z}}\left|\int_{I_{\mathrm{BVP}}}\big(-V(y)\big)_+^{1/2} dy - \pi(k+1/2)\right| \le \overline{C}\lambda^{-1}$. *Then*

(A) $|H(x)| \le \lambda^{-N}$ *if* x *lies to the left of* I.

(B) $(Av_I|H|^2)^{1/2} \le C_*$.

(C) $|H(x)| \le C_*$ *if* x *lies to the right of* I.

The constants C_*, $\overline{C}$ *depend only on* ε, K, N, c, c', C_α.

Remark. Again, the precise exponents in Case I (B), (C) are irrelevant to us, and are surely not optimal.

C. The Density for Degenerate One-dimensional Potentials II

In this section we give (very) crude results for the density without making any polynomial growth assumptions on the weight functions $S(x)$, $B(x)$ or the interval I. These results will be used later for ODE arising from three-dimensional problems, with angular momentum ℓ in the range [Large Constant, Z^ε]. The precise formulation is as follows.

Set-Up. We are given a potential $V(x)$ defined on a (possibly unbounded) interval I_{BVP}; positive functions $S(x)$, $B(x)$, defined on a subinterval $I \subset I_{\text{BVP}}$; a point $x_{\text{crit}} \in I_{\text{BVP}}$; an energy $E_{\text{crit}} \le 0$; and a number δ strictly between 0 and 1.

Assumptions

($\overline{\text{Z0}}$) For $x, y \in I$ with $|x-y| < cB(x)$, we have $c < \frac{B(y)}{B(x)} < C$ and $c < \frac{S(y)}{S(x)} < C$, and $|I| > cB(x)$.

($\overline{\text{Z1}}$) For $x \in I$ and $\alpha \ge 0$ we have $\left|\left(\frac{d}{dx}\right)^\alpha V(x)\right| \le C_\alpha S(x) B^{-\alpha}(x)$.

($\overline{\text{Z2}}$) For $E_{\text{crit}} \le E \le 0$, the set $\{x \in I_{\text{BVP}} \mid V(x) \le E\}$ is a non-empty interval $(x_{\text{left}}(E), x_{\text{rt}}(E))$ contained in I, with $\text{dist}(x_{\text{left}}(E), \partial I) > cB(x_{\text{left}}(E))$ and $\text{dist}\,(x_{\text{rt}}(E), \partial I) > cB(x_{\text{rt}}(E))$.

($\overline{\text{Z3}}$) For $E_{\text{crit}} \le E \le 0$, we have $-V'(x) \ge cS(x)B^{-1}(x)$ for $x \in [x_{\text{left}}(E), x_{\text{left}}(E) + c_1 B(x_{\text{left}}(E))]$ and $+V'(x) \ge cS(x)B^{-1}(x)$ for $x \in [x_{\text{rt}}(E) - c_1 B(x_{\text{rt}}(E)), x_{\text{rt}}(E)]$.

($\overline{\text{Z4}}$) For $E_{\text{crit}} \le E \le 0$, we have $cS(x) < E - V(x) < CS(x)$ for $x \in [x_{\text{left}}(E) +$

$c_1 B(x_{\text{left}}(E)), x_{\text{rt}}(E) - c_1 B(x_{\text{rt}}(E))]$

($\overline{Z5}$) $V(x)$ is decreasing and C^∞ on $I_{\text{BVP}}^{\text{interior}} \cap (-\infty, x_{\text{left}}(0)]$.

($\overline{Z6}$) For $E_{\text{crit}} \le E \le 0$, we have $x_{\text{left}}(E) + cB(x_{\text{left}}(E)) \le x_{\text{crit}}$.

($\overline{Z7}$) For $E_{\text{crit}} \le E \le 0$, we have

$$\int_{I_{\text{BVP}} \cap (-\infty, x_{\text{crit}}]} \left(E - V(t)\right)_+^{-1/2} dt \le \delta \int_{I_{\text{BVP}}} \left(E - V(t)\right)_+^{-1/2} dt$$

($\overline{Z8}$) $\Lambda \equiv \left(\int_{x_{\text{left}}(0)}^{x_{\text{rt}}(0)} \frac{dx}{\lambda(x) B(x)} \right)^{-1}$ is greater than a certain large, positive number determined by c, C, c_1, C_α above.

Here, $\lambda(x) = S^{1/2}(x) B(x)$ as usual.

If $\delta << 1$, then assumption ($\overline{Z7}$) says that in the semiclassical approximation, eigenfunctions $u_k(x)$ with eigenvalues $E_k \in [E_{\text{crit}}, 0]$ are almost entirely concentrated in $(x_{\text{crit}}, \infty) \cap I_{\text{BVP}}$. We want to show that the true density

$$\rho(x) = \sum_{E_k \le 0} |u_k(x)|^2$$

is then highly concentrated in the same interval. Here, E_k and $u_k(x)$ are the eigenvalues and (normalized) eigenfunctions of $-\frac{d^2}{dx^2} + V(x)$ with Dirichlet boundary conditions on I_{BVP}. The precise result is as follows.

Second Degenerate Density Lemma. *Assume ($\overline{Z0}$)… ($\overline{Z8}$). Then*

$$\int_{I_{\text{BVP}} \cap (-\infty, x_{\text{crit}}]} \rho(x) dx \le C_\# + C_\# \delta \int_{I_{\text{BVP}}} \left(-V(x)\right)_+^{1/2} dx + C_\# \int_{I_{\text{BVP}}} \left(E_{\text{crit}} - V(x)\right)_+^{1/2} dx$$

and $\int_{I_{\text{BVP}}} \rho(x) dx \le C_\# + C_\# \int_{I_{\text{BVP}}} \left(-V(x)\right)_+^{1/2} dx$, *with* $C_\#$ *depending only on* c, C, c_1, C_α *in ($\overline{Z0}$)… ($\overline{Z8}$).*

The Density for Degenerate One-Dimensional Potentials III

The results in this section are for application to three-dimensional problems, with angular momentum ℓ in the range $[1,\ \text{Large Constant}\,]$. Our setting is as follows.

We are given a potential $V(x)$, smooth on $(0,\infty)$. We take $B(x)=x$, and let $S(x)$ be a positive function on $I=[x_0,x_1]\subset(0,\infty)$. As usual, we set $\lambda(x)=S^{1/2}(x)B(x)$ on I. In addition to x_0, x_1, we are given other points x_{small}, x_{big}, x_{crit}, $x_*\in(0,\infty)$, with

$$0<x_{\text{small}}<\frac{1}{2}x_0\ ,\ 2x_0<x_{\text{crit}}<\frac{1}{2}x_*\ ,\ x_*<\frac{1}{16}x_1\ ,\ 2x_1<x_{\text{big}}\ . \tag{1}$$

Set $H=-\frac{d^2}{dx^2}+V(x)$ on $(0,\infty)$ with Dirichlet boundary conditions. Let E_k, $u_k(x)$ be the eigenvalues and (normalized) eigenfunctions of H. Define the density $\rho(x)$ as usual by $\rho(x)=\sum\limits_{E_k\le 0}|u_k(x)|^2$.

Our goal is to make a (very crude) estimate of $\int_0^{x_{\text{crit}}}\rho(x)dx$. In addition to (1), we make the following assumptions.

Hypotheses

(Z$\hat{0}$) If $x,y\in I$ and $|x-y|<\frac{1}{2}B(x)$, then $c<S(y)/S(x)<C$.

(Z$\hat{1}$) If $x\in I$, then $\left|\left(\frac{d}{dx}\right)^\alpha V(x)\right|\le C_\alpha S(x)B^{-\alpha}(x)$.

(Z$\hat{2}$) If $x\in I$, then $V(x)<-cS(x)$ and $V'(x)>cS(x)B^{-1}(x)$.

(Z$\hat{3}$) $\Lambda=\left(\int_I\frac{dx}{\lambda(x)B(x)}\right)^{-1}$ is greater than a certain large, positive number determined by c, C, C_α in (Z$\hat{0}$)…(Z$\hat{2}$).

(Z$\hat{4}$) For $x\in(0,x_{\text{small}}]$ we have $V(x)\ge\underline{c}x_0^{-2}$

(Z$\hat{5}$) For $x\in[x_{\text{small}},x_0]$ we have $|V(x)|\le\underline{C}x_0^{-2}$

(Z$\hat{6}$) We have $x_{\text{big}}<\underline{C}x_1$ and $V(x)$ is increasing in $[x_1,x_{\text{big}}]$.

(Z$\hat{7}$) For $x\in\left[\frac{x_1}{8},x_{\text{big}}\right]$, we have $|V(x)|\le\underline{C}x_1^{-2}$.

(Z$\hat{8}$) For $x\in[x_{\text{big}},\infty)$, we have $V(x)\ge 0$.

(Z$\hat{9}$) For $E\in[V(x_*),0]$ we have

$$\int_{x_0}^{x_{\text{crit}}}\big(E-V(x)\big)^{-1/2}dx\le\delta\cdot\int_{x_0}^{\frac{1}{2}x_*}\big(E-V(x)\big)^{-1/2}dx.$$

When $\delta << 1$ hypothesis $(\hat{Z9})$ shows that in the semiclassical approximation, most of the L^2-norm of an eigenfunction $u_k(x)$ with $E_k \in [V(x_*), 0]$ is concentrated outside of $(0, x_{\text{crit}}]$.

Third Degenerate Density Lemma. *Assume (1) and $(\hat{Z0})\ldots(\hat{Z9})$. Set $E_{\text{crit}} = V(x_*)$. Then*

$$\int_0^{x_{\text{crit}}} \rho(x)dx \le C_* + C_*\delta \int_0^\infty \left(-V(x)\right)_+^{1/2} dx + C_* \int_0^\infty \left(E_{\text{crit}} - V(x)\right)_+^{1/2} dx$$

and

$$\int_0^\infty \rho(x)dx \le C_* + C_* \int_0^\infty \left(-V(x)\right)_+^{1/2} dx$$

with C_* depending only on c, C, C_α, $\underline{c}$, $\underline{C}$, in $(\hat{Z0})\ldots(\hat{Z9})$.

E. The Density for Degenerate One-Dimensional Potentials IV

The results in this section will be used to handle angular momentum $\ell = 0$ in three-dimensional problems. Our setting is as follows.

We are given a smooth potential $V(x)$ on $(0,\infty)$. We take $B(x) = x$, and let $S(x)$ be a positive function on $I = [x_0, x_1] \subset (0,\infty)$. Let $\lambda(x) = S^{1/2}(x)B(x)$ as usual. We are given x_{crit}, x_*, x_{big}, satisfying

(1) $$16x_0 < x_{\text{crit}} \ , 16x_{\text{crit}} < x_* \ , 16x_* < x_1 \ , 16x_1 < x_{\text{big}} \ .$$

Set $H = -\frac{d^2}{dx^2} + V(x)$ on $(0,\infty)$, with Dirichlet boundary conditions. Let E_k, $u_k(x)$ be the eigenvalues and (normalized) eigenfunctions of H. Define the density $\rho(x)$ as usual by

$$\rho(x) = \sum_{E_k \le 0} |u_k(x)|^2 \ .$$

Our goal is to make a crude estimate of $\int_0^{x_{\text{crit}}} \rho(x)dx$. In addition to (1), we make the following assumptions.

Hypotheses.

(Z0†) If $x, y \in I$ and $|x-y| < \frac{1}{2}B(x)$, then $c < S(y)/S(x) < C$.

(Z1†) If $x \in I$ and $\alpha \geq 0$, then $\left|\left(\frac{d}{dx}\right)^\alpha V(x)\right| \leq C_\alpha S(x) B^{-\alpha}(x)$.

(Z2†) If $x \in I$, then $V(x) < -cS(x)$ and $V'(x) > cS(x)B^{-1}(x)$.

(Z3†) $\Lambda = \left(\int_I \frac{dx}{\lambda(x)B(x)}\right)^{-1}$ is greater than a certain large, positive number determined by c, C, C_α in (Z0†)...(Z2†).

(Z4†) $|V(x)| \leq \underline{C}/(x_0 x)$ for $x \in (0, x_0]$.

(Z5†) $V(x)$ is increasing and negative in $[\frac{x_1}{8}, x_{\text{big}}]$, and satisfies there $|V(x)| < \underline{C} x_1^{-2}$. Also, $x_{\text{big}} < \underline{C} x_1$.

(Z6†) $V(x) \geq -10^{-9} x^{-2}$ for $x \in [x_{\text{big}}, \infty)$.

(Z7†) For $E \in [V(x_*), 0]$, we have

$\int_{x_0}^{x_{\text{crit}}} \big(E - V(x)\big)^{-1/2} dx \leq \delta \cdot \int_{x_0}^{\frac{1}{2}x_*} \big(E - V(x)\big)^{-1/2} dx.$

As usual, (Z7†) says that certain eigenfunctions live mostly outside of $[x_0, x_{\text{crit}}]$ in the semiclassical approximation.

Fourth Degenerate Density Lemma. *Assume (1) and (Z0†)...(Z7†). Set $E_{\text{crit}} = V(x_*)$. Then*

$$\int_0^{x_{\text{crit}}} \rho(x)dx \leq C_* + C_*\delta \int_0^\infty \big(-V(x)\big)_+^{1/2} dx + C_* \int_0^\infty \big(E_{\text{crit}} - V(x)\big)_+^{1/2} dx$$

and $\int_0^\infty \rho(x)dx \leq C_* + C_* \int_0^\infty \big(-V(x)\big)_+^{1/2} dx$ with C_* depending only on c, C, C_α, $\underline{C}$ in (Z0†)...(Z7†).

F. Approximating Sums by Integrals

Separation of variables leads to a sum over all angular momenta ℓ. The following result lets us approximate such sums by integrals. For real numbers t, define:

$\chi_+(t) = k - t - \frac{1}{2}$ for k the smallest integer $\geq t$;

$\chi_-(t) = t - k - \frac{1}{2}$ for k the largest integer $\leq t$;

$\tilde{\chi}(t) = |t-k-\frac{1}{2}|^2 - \frac{1}{12}$ for an integer k that minimizes $|t-k-\frac{1}{2}|$.

Lemma on Riemann Sums. *Let $f(t)$, $\sigma(t)$, $\tau(t)$ be defined on a non–empty interval $[a,b]$. Suppose $\sigma(t) > 0$, $\tau(t) \geq 1$ in $[a,b]$; and assume that whenever $t_1, t_2 \in [a,b]$ with $|t_1 - t_2| < c\tau(t_1)$, we have $c < \frac{\tau(t_2)}{\tau(t_1)} < C$ and $c < \frac{\sigma(t_2)}{\sigma(t_1)} < C$. Finally assume $|(\frac{d}{dt})^m f(t)| \leq C_m \sigma(t)\tau^{-m}(t)$ for $t \in [a,b]$. Then $\sum\limits_{k\in\mathbb{Z}\cap[a,b]} f(k) = \int\limits_a^b f(t)dt - f(b)\chi_-(b) - f(a)\chi_+(a) + \frac{1}{2}f'(b)\tilde{\chi}(b) - \frac{1}{2}f'(a)\tilde{\chi}(a) +$ Error with $|\text{Error}| \leq C'\sigma(a)\tau^{-2}(a) + C'\sigma(b)\tau^{-2}(b) + C'_N \int_a^b \sigma(t)\tau^{-N}(t)dt$. Here, C' depends only on c, C, C_m; and C'_N depends only on c, C, C_m, N. If $f(t) = 0$ to infinite order at $t = a$, then we have the sharper estimate $|\text{Error}| \leq C'\sigma(b)\tau^{-2}(b) + C'_N \int_a^b \sigma(t)\tau^{-N}(t)dt$, with C', C'_N as before. Similarly, if $f(t) = 0$ to infinite order at $t = b$, then $|\text{Error}| \leq C'\sigma(a)\tau^{-2}(a) + C'_N \int_a^b \sigma(t)\tau^{-N}(t)dt$. If $f(t) = 0$ to infinite order at both $t = a$ and $t = b$, then $|\text{Error}| \leq C'_N \int\limits_a^b \sigma(t)\tau^{-N}(t)dt$.*

Separation of Variables

Our plan is to apply separation of variables to reduce spherically symmetric PDE problems to our known ODE theorems. Let $V(r)$ be a potential on $(0,\infty)$, and let $H=-\Delta+V(x)$ on $\mathbb{R}^3$, where we abuse notation by writing $V(x)$ for $V(|x|)$. Our goal, here and in [FS7], is to understand the eigenvalue sum

$$\operatorname{sneg}(H)=\sum_{E_k\le 0}E_k$$

and the density

$$\rho(x)=\sum_{E_k\le 0}|\psi_k(x)|^2\ ,$$

where E_k, $\psi_k(x)$ denote the eigenvalues and normalized eigenfunctions of H.

For $\ell\ge 0$, form the potential $V_\ell(r)=\frac{\ell(\ell+1)}{r^2}+V(r)$, and let H_ℓ denote the ordinary differential operator $H_\ell=-\frac{d^2}{dr^2}+V_\ell(r)$ on $(0,\infty)$, with Dirichlet boundary conditions. Let $E_{n,\ell}$, $u_{n\ell}(r)$ $\big(1\le n\le n_{\max}(\ell)\big)$ be the eigenvalues and normalized eigenfunctions of H_ℓ. The eigenvalue sum and density for H_ℓ are

$$\operatorname{sneg}(H_\ell)=\sum_{E_{n,\ell}\le 0}E_{n\ell}$$

$$\rho_\ell(r)=\sum_{E_{n\ell}\le 0}|u_{n\ell}(r)|^2\ .$$

Introduce the spherical harmonics $Y_{\ell m}(w)$ $(m=1,\dots,2\ell+1)$ defined on the unit sphere S^2 in $\mathbb{R}^3$. We take the $Y_{\ell m}(w)$ orthonormal in $L^2(S^2)$ with respect to surface area. Then the eigenvalues and normalized eigenfunctions of H are

$$E_{n\ell}\ ,\ \psi_{n\ell m}(rw)=r^{-1}u_{n\ell}(r)Y_{\ell m}(w)\quad \text{for } r>0\ ,\ w\in S^2\ .$$

Since $\sum_m|Y_{\ell m}(w)|^2=\frac{2\ell+1}{4\pi}$ on S^2, it follows that

$$\operatorname{sneg}(H)=\sum_{\ell\ge 0}(2\ell+1)\operatorname{sneg}(H_\ell)\ ,\quad \text{and}$$

$$4\pi r^2\rho(rw)=\sum_{\ell\ge 0}(2\ell+1)\rho_\ell(r)\quad \text{for}\quad r>0\ ,\ w\in S^2\ .$$

We will control $\operatorname{sneg}(H_\ell)$ and $\rho_\ell(r)$ by using our ODE results, and then perform the sum over ℓ.

The potentials of interest to us arise by rescaling the potential

$$V_\Omega(x) = \frac{\Omega}{x^2} - \frac{y(x)}{x} \quad x \in (0,\infty)\ ,\ \Omega \in [0,\infty)\ , \tag{1}$$

where $y(x)$ is the solution of the Thomas-Fermi differential equation

$$\frac{d^2}{dx^2} y(x) = y^{3/2}(x) \cdot x^{-1/2}\ ,\ y(0) = 1\ ,\ y(\infty) = 0\ . \tag{2}$$

The basic properties of (2) are well-known. In particular, Hille [Hi] contains the following results.

Lemma 1. *$y(x)$ is smooth and strictly between 0 and 1 for $x \in (0,\infty)$, while $y'(x)$ is bounded and negative on $(0,\infty)$. For x small, $y(x)$ has a convergent series expansion of the form*

$$y(x) = 1 - wx + \sum_{k\geq 3} w_k x^{k/2}\ ,\ \textit{with } w > 0 \textit{ and } w_k \textit{ real}\ . \tag{3}$$

For x large, $y(x)$ has a convergent series expansion

$$y(x) = 144\ x^{-3}\big(1 + \sum_{k\geq 1} b_k x^{-k\gamma}\big) \quad \textit{with } \gamma = \frac{1}{2}(\sqrt{73} - 7)\ . \tag{4}$$

We seldom need (3) and (4) in full strength. Instead, we will just use the following

Corollary. *Given $\eta > 0$, there exist constants $0 < k_1(\eta) < K_2(\eta)$ such that*

$$\textit{If } 0 < \overline{x} \leq k_1(\eta)\ ,\ \textit{then } \Big|\Big(\frac{d}{dt}\Big)^\alpha \big\{y(\overline{x}t) - 1\big\}\Big| < \eta \quad \textit{for } 0 \leq \alpha \leq 4 \textit{ and } \frac{1}{2} \leq t \leq 2\ . \tag{5}$$

$$\textit{If } \overline{x} \geq K_2(\eta)\ ,\ \textit{then } \Big|\Big(\frac{d}{dt}\Big)^\alpha \Big\{\frac{(\overline{x}t)^3}{144} y(\overline{x}t) - 1\Big\}\Big| < \eta \quad \textit{for } 0 \leq \alpha \leq 4 \textit{ and } \frac{1}{2} \leq t \leq 2\ . \tag{6}$$

Regarding $V_\Omega(x)$, the following results may be found, for instance, in Hughes [Hu], pp. 235–236.

Let $\overline{\Omega} = \max_{x>0}\big(xy(x)\big) > 0$. Thus, $V_\Omega \geq 0$ for $\Omega \geq \overline{\Omega}$.

Lemma 2. *Let $\Omega \in (0, \overline{\Omega})$. Then V_Ω has exactly two zeros $x_1(\Omega)$ and $x_2(\Omega)$, and two critical points $x_0(\Omega)$, $x_m(\Omega)$, and these points may be taken to satisfy*

(7) $0 < x_1(\Omega) < x_0(\Omega) < x_2(\Omega) < x_m(\Omega)$, *and* $V_\Omega\big(x_0(\Omega)\big) < 0 < V_\Omega\big(x_m(\Omega)\big)$.

Lemma 3. *Given $\varepsilon > 0$, there exist positive constants $c_i(\varepsilon)$ $(0 \leq i \leq 5)$ with the following properties: For $\Omega \in (\varepsilon, \overline{\Omega})$, we have*

(8)
$$V_\Omega''\big(x_0(\Omega)\big) > c_0(\varepsilon)$$

(9)
$$\Big|\Big(\frac{d}{dx}\Big)^k V_\Omega(x)\Big| < c_k(\varepsilon) \quad \textit{for} \quad 1 \leq k \leq 3 \quad \textit{and } x \in \Big[\frac{\Omega}{10}\ , 2x_2(\Omega)\Big]$$

(10)
$$V_\Omega'(x) < -c_4(\varepsilon) \quad \textit{for } x \in \Big[\frac{\Omega}{10}\ , x_0(\Omega) - c_5(\varepsilon)\Big]$$

(11)
$$V_\Omega'(x) > c_4(\varepsilon) \textit{ for } x \in \Big[x_0(\Omega) + c_5(\varepsilon)\ , \frac{x_2(\Omega) + x_m(\Omega)}{2}\Big]$$

(12) *For* $|x - x_0(\Omega)| \leq c_5(\varepsilon)$ *, we have*

$$\frac{9}{20} V_\Omega''\big(x_0(\Omega)\big) \cdot \big(x - x_0(\Omega)\big)^2 \leq V_\Omega(x) - V_\Omega\big(x_0(\Omega)\big)$$
$$\leq \frac{11}{20} V_\Omega''\big(x_0(\Omega)\big) \cdot \big(x - x_0(\Omega)\big)^2 \ .$$

Immediately from Lemmas 1, 2, 3, we see that $V_\Omega'(x) < 0$ for $x < x_0(\Omega)$, and that $V_\Omega''(x_m(\Omega)) \leq 0$. In fact, Lemma 2 shows that V_Ω' cannot change sign in $(0, x_0(\Omega))$, and Lemma 3 gives $V_\Omega'(x_1(\Omega)) < 0$. Therefore, $V_\Omega' < 0$ on $(0, x_0(\Omega))$. Moreover, we see from Lemmas 2 and 3 that V_Ω cannot change sign in $(x_2(\Omega), \infty)$, and that

$V_\Omega(x_2(\Omega)) = 0$, $V'_\Omega(x_2(\Omega)) > 0$. Therefore, V_Ω is a positive, smooth function on $I = (x_2(\Omega), \infty)$, and V_Ω tends to zero at the endpoints of I. Consequently, $V_\Omega\,|_I$ assumes a maximum at some point $x_c(\Omega) \in I$. In particular, $V''_\Omega(x_c(\Omega)) \leq 0$, $V'_\Omega(x_c(\Omega)) = 0$, $x_c(\Omega) > x_2(\Omega)$. These last two conditions and Lemma 2 show that $x_c(\Omega) = x_m(\Omega)$. Thus, $V''_\Omega(x_m(\Omega)) \leq 0$, as asserted.

Unfortunately, we will need to use a long list of additional elementary properties of $V_\Omega(x)$. These properties are surely well-known to anyone interested in atoms, but we don't know where to find them in the literature. Hence, we will prove them here, as consequences of Lemmas 1, 2, 3. Specifically, we will need the following result.

Main Lemma on the Thomas-Fermi Potential. *Let* $S(x) = \min\{x^{-1}, x^{-4}\}$. *There exist universal constants* $\overline{c}$, c_1, c_2, $\hat{c}$, $\hat{C}$, $C_\alpha > 0$ *for which the following properties hold.*

I. *Suppose* $0 < \Omega \leq (1-\overline{c})\overline{\Omega}$. *Then we have the following.*

A. *The Size and Sign of* $V_\Omega(x)$

(13) $$\hat{c}\Omega x^{-2} < V_\Omega(x) < \hat{C}\Omega x^{-2} \quad \textit{for} \quad x \in \big(0, (1-c_1)x_1(\Omega)\big]$$

(14)
$$\hat{c}S\big(x_1(\Omega)\big)\cdot\big(x_1(\Omega)\big)^{-1}\big(x_1(\Omega)-x\big) \leq V_\Omega(x) \leq \hat{C}S\big(x_1(\Omega)\big)\cdot\big(x_1(\Omega)\big)^{-1}\big(x_1(\Omega)-x\big)$$
$$\textit{for } x \in \big[(1-c_1)x_1(\Omega), x_1(\Omega)\big]$$

(15)
$$\hat{c}S\big(x_1(\Omega)\big)\cdot\big(x_1(\Omega)\big)^{-1}\big(x-x_1(\Omega)\big) \leq -V_\Omega(x) \leq \hat{C}S\big(x_1(\Omega)\big)\cdot\big(x_1(\Omega)\big)^{-1}\big(x-x_1(\Omega)\big)$$
$$\textit{for } x \in \big[x_1(\Omega), (1+c_1)x_1(\Omega)\big] \blacksquare$$

(16) $$\hat{c}S(x) < -V_\Omega(x) < \hat{C}S(x) \quad \textit{for } x \in \big[(1+c_1)x_1(\Omega), (1-c_1)x_2(\Omega)\big]$$

(17)

$$\hat{c}S\big(x_2(\Omega)\big)\big(x_2(\Omega)\big)^{-1}\big(x_2(\Omega)-x\big) \le -V_\Omega(x) \le \hat{C}S\big(x_2(\Omega)\big)\big(x_2(\Omega)\big)^{-1}\big(x_2(\Omega)-x\big)$$
$$\textit{for } x \in \big[(1-c_1)x_2(\Omega), x_2(\Omega)\big] \ .$$

(18)

$$\hat{c}S\big(x_2(\Omega)\big)\big(x_2(\Omega)\big)^{-1}\big(x-x_2(\Omega)\big) \le V_\Omega(x) \le \hat{C}S\big(x_2(\Omega)\big)\big(x_2(\Omega)\big)^{-1}\big(x-x_2(\Omega)\big)$$
$$\textit{for } x \in \big[x_2(\Omega), (1+c_1)x_2(\Omega)\big]$$

(19) $$\hat{c}\Omega x^{-2} < V_\Omega(x) < \hat{C}\Omega x^{-2} \quad \textit{for } x \in \big[(1+c_1)x_2(\Omega), \infty\big) \ .$$

B. *The Size and Sign of Derivatives of* $V_\Omega(x)$

(20) $$\hat{c}\Omega x^{-3} < -V'_\Omega(x) < \hat{C}\Omega x^{-3} \quad \textit{for } x \in \big(0, (1-c_1)x_0(\Omega)\big]$$

(21)

$$\hat{c}S(x)x^{-2} < V''_\Omega(x) < \hat{C}S(x)x^{-2} \quad \textit{for } x \in \big[(1-c_1)x_0(\Omega), (1+c_1)x_0(\Omega)\big] \ ,$$
$$\textit{and } V'_\Omega\big(x_0(\Omega)\big) = 0 \ .$$

(22) $$\hat{c}S(x)x^{-1} < V'_\Omega(x) < \hat{C}S(x)x^{-1} \quad \textit{for } x \in \big[(1+c_1)x_0(\Omega), (1+c_1)x_2(\Omega)\big]$$

(23) $$\Big|\big(\frac{d}{dx}\big)^\alpha V_\Omega(x)\Big| \le C_\alpha S(x)x^{-\alpha} \quad \textit{for } x \in \big[(1-c_1)x_1(\Omega), (1+c_1)x_2(\Omega)\big] \ .$$

C. *The Zeros and Critical Points of* $V_\Omega(x)$

(24) $$\hat{c}\Omega < x_1(\Omega) < x_0(\Omega) < \hat{C}\Omega \ , \quad x_0(\Omega) - x_1(\Omega) > \hat{c}\Omega$$

(25) $$\hat{c}\Omega^{-1/2} < x_2(\Omega) < x_m(\Omega) < \hat{C}\Omega^{-1/2} \ , \quad x_m(\Omega) - x_2(\Omega) > \hat{c}\Omega^{-1/2}$$

(26) $$x_m(\Omega) > (1+2c_1)x_2(\Omega) \quad \textit{and} \quad x_1(\Omega) < (1-c_1)x_0(\Omega)$$
$$\textit{and} \quad x_0(\Omega) < (1-2c_1)x_2(\Omega) \ .$$

II. *Suppose* $(1-\overline{c})\overline{\Omega} \le \Omega < \overline{\Omega}$. *Then we have the following.*

(27)
$$\Big|\big(\frac{d}{dx}\big)^{\alpha} V_{\Omega}(x)\Big| \le C_{\alpha} S(x) x^{-\alpha} \quad \textit{and} \quad \hat{c} S(x) x^{-2} < V''_{\Omega}(x) < \hat{C} S(x) x^{-2}$$
$$\textit{for } x \in \big[(1-c_2)x_0(\Omega), (1+c_2)x_0(\Omega)\big] \ .$$

(28)
$$V_{\Omega}(x) > \hat{c}\Omega x^{-2} \quad \textit{for} \quad x \notin \big[(1-c_2)x_0(\Omega), (1+c_2)x_0(\Omega)\big] \ .$$

(29)
$$\hat{c}(\overline{\Omega}-\Omega) < -V_{\Omega}\big(x_0(\Omega)\big) < \hat{C}(\overline{\Omega}-\Omega) \ .$$

The rest of this section is devoted to proving the above Main Lemma. We look separately at the three regions $0 < \Omega < \varepsilon$, $\varepsilon \le \Omega \le \overline{\Omega} - \varepsilon$, $\overline{\Omega} - \varepsilon \le \Omega < \overline{\Omega}$, for a small, positive ε to be picked later. We begin by proving the following preliminary result.

Lemma 4. *The functions* $x_1(\Omega)$, $x_2(\Omega)$, $x_0(\Omega)$ *are smooth on* $(0,\overline{\Omega})$, *and* $x_m(\Omega)$ *is continuous on* $(0,\overline{\Omega})$.

Proof. To handle $x_0(\Omega)$, $x_1(\Omega)$, $x_2(\Omega)$, we need only apply the implicit function theorem, since $V_{\Omega}(x)$ is smooth on $(0,\infty)\times(0,\infty)$ and we know that $V_{\Omega}\big(x_1(\Omega)\big) = 0$, $V'_{\Omega}\big(x_1(\Omega)\big) < 0$; $V_{\Omega}\big(x_2(\Omega)\big) = 0$, $V'_{\Omega}\big(x_2(\Omega)\big) > 0$; $V'_{\Omega}\big(x_0(\Omega)\big) = 0$, $V''_{\Omega}\big(x_0(\Omega)\big) > 0$ by Lemmas 2 and 3. For $x_m(\Omega)$ we need a different argument, because Lemmas 2 and 3 do not assert that $V''_{\Omega}\big(x_m(\Omega)\big)$ is strictly negative. We proceed as follows.

We know from (6) that $\big|\frac{d}{dx}\big(y(x)x^{-1}\big)\big| \le Cx^{-5}$ for $x \ge C$, where $C > 0$ is a large, universal constant. Hence, $V'_{\Omega}(x) \le -2\Omega x^{-3} + Cx^{-5} < 0$ for $x > \max\big\{C, \big(\frac{C}{2\Omega}\big)^{1/2}\big\}$. Since $V'_{\Omega}\big(x_m(\Omega)\big) = 0$, it follows that

(30)
$$x_m(\Omega) \le \max\Big\{C, \big(\frac{C}{2\Omega}\big)^{1/2}\Big\} \quad \text{for } \Omega \in (0,\overline{\Omega}) \ .$$

Now we suppose $x_m(\Omega)$ discontinuous and derive a contradiction. If $x_m(\Omega)$ is discontinuous, then we can find $\Omega_\nu \to \hat{\Omega}$ with $\hat{\Omega} \in (0,\infty)$ and $x_m(\Omega_\nu) \nrightarrow x_m(\hat{\Omega})$.

The $x_m(\Omega_\nu)$ are positive, and (30) shows that they remain bounded. Hence, by passing to a subsequence, we may assume $x_m(\Omega_\nu) \to \hat{x}$ with $\hat{x} \neq x_m(\hat{\Omega})$. Since $x_m(\Omega_\nu) > x_2(\Omega_\nu)$ and $x_2(\Omega_\nu) \to x_2(\hat{\Omega}) > 0$ we know that $\hat{x}$ is strictly positive. Noting that $V'_{\Omega_\nu}\big(x_m(\Omega_\nu)\big) = 0$ and passing to the limit, we see that $V'_{\hat{\Omega}}(\hat{x}) = 0$. Therefore, $\hat{x} = x_m(\hat{\Omega})$ or $\hat{x} = x_0(\hat{\Omega})$, by Lemma 2. We know that $\hat{x} \neq x_m(\hat{\Omega})$, so $\hat{x} = x_0(\hat{\Omega})$. Hence, $V''_{\hat{\Omega}}(\hat{x}) > 0$, by Lemma 3. On the other hand, we have $V''_{\Omega_\nu}\big(x_m(\Omega_\nu)\big) \leq 0$. Passing to the limit, we find that $V''_{\hat{\Omega}}(\hat{x}) \leq 0$. Thus, $V''_{\hat{\Omega}}(\hat{x}) > 0$ and $V''_{\hat{\Omega}}(\hat{x}) \leq 0$. This contradiction completes the proof. $\square$

Lemma 5. *Given $\varepsilon > 0$ there exists $\delta > 0$ such that for every $c_1 \in (0, \delta)$ there exist $\hat{c}$, $\hat{C}$, C_α, depending only on ε and c_1, such that (13),…,(26) hold for all $\Omega \in [\varepsilon, \overline{\Omega} - \varepsilon]$.*

Proof. Let $c_A(\varepsilon)$, $c_B(\varepsilon)$, etc. denote positive constants depending only on ε. Similarly, let $c_A(\varepsilon, c_1)$, $c_B(\varepsilon, c_1)$ etc. denote positive constants depending only on ε and c_1.

Lemma 4 and (7) show that we can find $c_A(\varepsilon)$, $C_B(\varepsilon)$ so that the following properties hold.

(31) $$c_A(\varepsilon) < x_1(\Omega) < x_0(\Omega) < x_2(\Omega) < x_m(\Omega) < C_B(\varepsilon) \quad \text{for } \Omega \in [\varepsilon, \overline{\Omega} - \varepsilon]$$

(32) $$x_m(\Omega) > (1 + 2c_A(\varepsilon))x_2(\Omega) \quad \text{and}$$
$$x_0(\Omega) < (1 - 2c_A(\varepsilon))x_2(\Omega) \text{ and}$$
$$x_1(\Omega) < (1 - c_A(\varepsilon))x_0(\Omega) \quad \text{for } \Omega \in [\varepsilon, \overline{\Omega} - \varepsilon]\ .$$

Next, note that $-V'_\Omega(x)\big[S(x)x^{-1}\big]^{-1}$ is continuous on $F = \{(\Omega, x)\colon \Omega \in [\varepsilon, \overline{\Omega} - \varepsilon],\ \frac{1}{2}c_A(\varepsilon) \leq x \leq 2C_B(\varepsilon)\}$ and strictly positive for $x = x_1(\Omega)$. Therefore, for suitable constants $c_D(\varepsilon)$, $C_E(\varepsilon)$, $c_F(\varepsilon)$, we have

$$(33)\quad c_D(\varepsilon)S(x)x^{-1} < -V'_\Omega(x) < C_E(\varepsilon)S(x)x^{-1} \quad \text{for} \quad |x - x_1(\Omega)| \le c_F(\varepsilon)x_1(\Omega)\ ,\ \Omega \in [\varepsilon, \overline{\Omega} - \varepsilon]\ .$$

Similarly,

$$(34)\quad c_G(\varepsilon)S(x)x^{-1} < V'_\Omega(x) < C_H(\varepsilon)S(x)x^{-1} \quad \text{for } |x - x_2(\Omega)| \le c_I(\varepsilon)x_2(\Omega), \Omega \in [\varepsilon, \overline{\Omega} - \varepsilon]\ .$$

Again, since $V''_\Omega(x)[S(x)x^{-2}]^{-1}$ is continuous on F and strictly positive for $x = x_0(\Omega)$, we have

$$(35)\quad c_J(\varepsilon)S(x)x^{-2} < V''_\Omega(x) < C_K(\varepsilon)S(x)x^{-2} \quad \text{for } |x - x_0(\Omega)| \le c_L(\varepsilon)x_0(\Omega)\ ,\ \Omega \in [\varepsilon, \overline{\Omega} - \varepsilon]\ .$$

Now suppose we are given c_1 satisfying

$$(36)\qquad 0 < c_1 < \min\Big\{\frac{1}{10}, c_A(\varepsilon), c_F(\varepsilon), c_I(\varepsilon), c_L(\varepsilon)\Big\}\ .$$

Since $x_1(\Omega) > 0$, $x_2(\Omega) > 0$ are continuous, we can find $c_M(\varepsilon, c_1) < \varepsilon$ such that $\Omega \in [\varepsilon, \overline{\Omega} - \varepsilon]$, $|\tilde{\Omega} - \Omega| \le c_M(\varepsilon, c_1)$ imply $|x_i(\Omega) - x_i(\tilde{\Omega})| \le c_1 x_i(\Omega)$ $(i = 1, 2)$, so that $[x_1(\Omega)\cdot(1-c_1), x_2(\Omega)\cdot(1+c_1)] \supset [x_1(\tilde{\Omega}), x_2(\tilde{\Omega})]$. Set $\tilde{\Omega} = \Omega - c_M(\varepsilon, c_1)$. Since $V_\Omega(x) = c_M(\varepsilon, c_1)x^{-2} + V_{\tilde{\Omega}}(x)$ and $V_{\tilde{\Omega}}(x) > 0$ outside $[x_1(\tilde{\Omega}), x_2(\tilde{\Omega})]$, it follows that

$$(37)\qquad V_\Omega(x) \ge c_M(\varepsilon, c_1)x^{-2} \quad \text{for } x \le (1 - c_1)x_1(\Omega)\ ,\ \Omega \in [\varepsilon, \overline{\Omega} - \varepsilon]\ , \text{and}$$

$$(38)\qquad V_\Omega(x) \ge c_M(\varepsilon, c_1)x^{-2} \quad \text{for } x \ge (1 + c_1)x_2(\Omega)\ ,\ \Omega \in [\varepsilon, \overline{\Omega} - \varepsilon]\ .$$

Also, for all Ω, x, we have

$$(39)\qquad V_\Omega(x) = \Omega x^{-2} - y(x)x^{-1} < \Omega x^{-2}\ .$$

Equations (37), (38), (39) show that properties (13) and (19) hold for $\hat{c}$ small enough and $\hat{C}$ large enough, depending on c_1 and ε.

Next, note that $-V_\Omega(x)S^{-1}(x)$ is strictly positive and continuous on $\{(\Omega, x)\colon \Omega \in [\varepsilon, \overline{\Omega}-\varepsilon],\ (1+c_1)x_1(\Omega) \le x \le (1-c_1)x_2(\Omega)\}$. Hence,

$$c_N(\varepsilon, c_1)S(x) < -V_\Omega(x) < C_O(\varepsilon, c_1)S(x) \quad \text{for } (1+c_1)x_1(\Omega) \le x \le (1-c_1)x_2(\Omega)\ ,\ \Omega \in [\varepsilon, \overline{\Omega}-\varepsilon]\ .$$

This proves property (16) for $\hat{c}$ small enough and $\hat{C}$ large enough, depending on c_1 and ε.

Since $V\big(x_1(\Omega)\big) = 0$, properties (14) and (15) follow from (33) and (36), for $\hat{c}$ small enough and $\hat{C}$ large enough, depending on c_1 and ε. Similarly, properties (17) and (18) follow from (34) and (36).

Thus, we have verified properties (13)...(19).

Next, since $x_0(\Omega)$ is continuous, we can find $c_P(\varepsilon, c_1) < \varepsilon$ such that $\Omega \in [\varepsilon, \overline{\Omega}-\varepsilon]$ and $|\tilde{\Omega}-\Omega| \le c_P(\varepsilon, c_1)$ implies $|x_0(\Omega)-x_0(\tilde{\Omega})| < c_1 x_0(\Omega)$. Taking $\tilde{\Omega} = \Omega - c_P(\varepsilon, c_1)$, we obtain $x_0(\tilde{\Omega}) > (1-c_1)x_0(\Omega)$, so that $V'_{\tilde{\Omega}}(x) < 0$ for $x \le (1-c_1)x_0(\Omega)$. Since $V_\Omega(x) = c_P(\varepsilon, c_1)x^{-2} + V_{\tilde{\Omega}}(x)$, it follows that

$$V'_\Omega(x) < -2c_P(\varepsilon, c_1)x^{-3} \quad \text{for} \quad x \le (1-c_1)x_0(\Omega)\ ,\ \Omega \in [\varepsilon, \overline{\Omega}-\varepsilon]\ . \tag{40}$$

On the other hand, for $x \le (1-c_1)x_0(\Omega) \le x_0(\Omega) \le C_B(\varepsilon)$, we have

$$|V'_\Omega(x)| = |-2\Omega x^{-3} - y(x)x^{-2} + y'(x)x^{-1}| \le C_Q(\varepsilon)x^{-3}\ . \tag{41}$$

Estimates (40) and (41) imply property (20) for $\Omega \in [\varepsilon, \overline{\Omega}-\varepsilon]$, if $\hat{c}$ is small enough and $\hat{C}$ large enough, depending on c_1 and ε.

Property (21) follows at once from (35), (36), if $\hat{c}$ is small enough and $\hat{C}$ large enough, depending on c_1 and ε.

Next, note that $V'_\Omega(x)\cdot[S(x)x^{-1}]^{-1}$ is strictly positive and continuous on $\{(\Omega, x)\colon \Omega \in [\varepsilon, \overline{\Omega} - \varepsilon],\ (1 + c_1)x_0(\Omega) \le x \le (1 + c_1)x_2(\Omega)\}$, since $\big(x_0(\Omega), (1 + c_1)x_2(\Omega)\big] \subset \big(x_0(\Omega), x_m(\Omega)\big)$ by (32), (36). Therefore,

$$c_R(\varepsilon, c_1)S(x)x^{-1} < V'_\Omega(x) < C_S(\varepsilon, c_1)S(x)x^{-1}$$
$$\text{for } (1 + c_1)x_0(\Omega) \le x \le (1 + c_1)x_2(\Omega)\ ,\ \ \Omega \in [\varepsilon, \overline{\Omega} - \varepsilon]\ .$$

This proves property (22) for $\hat{c}$ small enough and $\hat{C}$ large enough, depending on c_1 and ε.

Next, since $\big[\big(\frac{d}{dx}\big)^\alpha V_\Omega(x)\big][S(x)x^{-\alpha}]^{-1}$ is continuous on $\big\{(\Omega, x)\colon \Omega \in [\varepsilon, \overline{\Omega} - \varepsilon]$ and $\frac{1}{2}x_1(\Omega) \le x \le 2x_2(\Omega)\big\}$, it follows that

$$\Big|\Big(\frac{d}{dx}\Big)^\alpha V_\Omega(x)\Big| \le C_\alpha(\varepsilon)S(x)x^{-\alpha} \quad \text{for } \frac{1}{2}x_1(\Omega) \le x \le 2x_2(\Omega)\ ,\ \ \Omega \in [\varepsilon, \overline{\Omega} - \varepsilon]\ .$$

This implies property (23), since $c_1 \le \frac{1}{10}$ by (36).

Finally, properties (24), (25), (26) follow from (31), (32), (36) if we take $\hat{c}$ small enough and $\hat{C}$ large enough, depending on c_1 and ε. Thus, we have verified properties (13)...(26). The proof of Lemma 5 is complete. □

Next, we study $\Omega \in (0, \varepsilon]$.

Lemma 6. *There exist positive universal constants ε_0, c_1, $\hat{c}$, $\hat{C}$, C_α for which properties (13)...(26) hold for all $\Omega \in (0, \varepsilon_0]$. We can take $c_1 = 10^{-2}$.*

Proof. We use k_1, K_2, etc. to denote positive, universal constants. We start by applying (5) and (6) with $\eta = 10^{-50}$. Thus, there exist constants $0 < k_1 < K_2$ such that

$$\text{(42)} \quad \Big|\Big(\frac{d}{dt}\Big)^\alpha \{y(xt) - 1\}\Big| < 10^{-50}$$
$$\text{for } 0 \le \alpha \le 4,\ \frac{1}{2} \le t \le 2,\ 0 < x \le k_1\ ; \quad \text{and}$$

$$(43)\qquad \Big|\big(\frac{d}{dt}\big)^{\alpha}\big\{\frac{(xt)^3 y(xt)}{144}-1\big\}\Big| < 10^{-50} \quad \text{for } 0\le\alpha\le 4,\ \frac{1}{2}\le t\le 2,\ x\ge K_2\ .$$

We may take $k_1 < 1 < K_2$.

In $[k_1, K_2]$, the function $-y(x)x^{-1}$ is negative and smooth, and its derivative is positive. Therefore, for suitable constants K_3, k_4, k_5, K_6, K^α, we have

$$(44)\qquad -K_3 S(x) < -y(x)x^{-1} < -2k_4 S(x) \quad \text{for} \quad k_1\le x\le K_2\ ;$$

$$(45)\qquad 2k_5 S(x)x^{-1} < -\frac{d}{dx}\big(y(x)x^{-1}\big) < K_6 S(x)x^{-1} \quad \text{for} \quad k_1\le x\le K_2\ ;$$

$$(46)\qquad \big|\big(\frac{d}{dx}\big)^{\alpha}(y(x)x^{-1})\big| \le K^\alpha S(x)x^{-\alpha} \quad \text{for} \quad \alpha\ge 0\ ,\ k_1\le x\le K_2\ .$$

Pick ε_0 in $(0, \frac{1}{10})$ so small that $0<\Omega\le 2\varepsilon_0$ implies

$$(47)\qquad \big|\frac{d}{dx}(\Omega x^{-2})\big| \le k_5 S(x)x^{-1} \quad \text{for } k_1\le x\le K_2\ ;$$

$$(48)\qquad |(\Omega x^{-2})| < k_4 S(x) \quad \text{for} \quad k_1\le x\le K_2\ ;$$

$$(49)\qquad 10\Omega < k_1\ ;$$

$$(50)\qquad \Omega^{-1/2} > K_2\ .$$

Then take $c_1 = 10^{-2}$. We will check that (13)...(26) hold for suitable universal constants $\hat{c}$, $\hat{C}$, C_α. We begin by locating $x_0(\Omega)$, $x_1(\Omega)$, $x_2(\Omega)$, $x_m(\Omega)$, for $0<\Omega\le\varepsilon_0$. Thus, fix $\Omega\in(0,\varepsilon_0]$.

Set $f(t)=\Omega V_\Omega(\Omega t) = [t^{-2}-t^{-1}-(y(\Omega t)-1)t^{-1}]$. Applying (42) and (49), we see that $f(1-10^{-49})>0>f(1+10^{-49})$. Hence there is a point $\tilde{x}_1(\Omega)$ satisfying

$$(51)\qquad |\tilde{x}_1(\Omega)-\Omega| < 10^{-49}\Omega \quad \text{and} \quad V_\Omega(\tilde{x}_1(\Omega)) = 0\ .$$

Next, set

$$f(t) = 4\Omega^2 V_\Omega'(2\Omega t) = -t^{-3} + t^{-2} + [y(2\Omega t) - 1]t^{-2} - t^{-1}\frac{d}{dt}\{y(2\Omega t) - 1\} \ .$$

Applying (42) and (49) again, we see that $f(1-10^{-49}) < 0 < f(1+10^{-49})$. Hence, there is a point $\tilde{x}_0(\Omega)$ satisfying

$$|\tilde{x}_0(\Omega) - 2\Omega| < 2\cdot 10^{-49}\Omega \quad \text{and} \quad V_\Omega'\big(\tilde{x}_0(\Omega)\big) = 0 \ . \tag{52}$$

Similarly, set $f(t) = 144\Omega^{-2}V_\Omega(12\Omega^{-1/2}t) = t^{-2} - t^{-4} - t^{-4}\left\{\frac{(12\Omega^{-1/2}t)^3 y(12\Omega^{-1/2}t)}{144} - 1\right\}$. Applying (43) and (50), we see that $f(1-10^{-49}) < 0 < f(1+10^{-49})$. Hence, there is a point $\tilde{x}_2(\Omega)$ satisfying

$$|\tilde{x}_2(\Omega) - 12\Omega^{-1/2}| < 12\cdot 10^{-49}\Omega^{-1/2} \quad \text{and} \quad V_\Omega\big(\tilde{x}_2(\Omega)\big) = 0 \ . \tag{53}$$

Next, set

$$\begin{aligned} f(t) &= 144\Omega^{-2}\frac{d}{dt}V_\Omega(12\sqrt{2}\Omega^{-1/2}t) \\ &= -t^{-3} + t^{-5} + t^{-5}\left[\frac{(12\sqrt{2}\,\Omega^{-1/2}t)^3 y(12\sqrt{2}\,\Omega^{-1/2}t)}{144} - 1\right] \\ &\qquad - \frac{1}{4}t^{-4}\frac{d}{dt}\left\{\frac{(12\sqrt{2}\,\Omega^{-1/2}t)^3 y(12\sqrt{2}\,\Omega^{-1/2}t)}{144} - 1\right\} \ . \end{aligned}$$

Applying (43) and (50) again, we see that $f(1-10^{-49}) > 0 > f(1+10^{-49})$. Hence there is a point $\tilde{x}_m(\Omega)$ satisfying

$$|\tilde{x}_m(\Omega) - 12\sqrt{2}\,\Omega^{-1/2}| < 10^{-49}\cdot 12\sqrt{2}\,\Omega^{-1/2} \quad \text{and} \quad V_\Omega'\big(\tilde{x}_m(\Omega)\big) = 0 \ . \tag{54}$$

Since $\Omega \le \varepsilon_0 \le \frac{1}{10}$, equations (51)...(54) show that $0 < \tilde{x}_1(\Omega) < \tilde{x}_0(\Omega) < \tilde{x}_2(\Omega) < \tilde{x}_m(\Omega)$. Since $\tilde{x}_1(\Omega)$, $\tilde{x}_2(\Omega)$ are zeros of V_Ω, and $\tilde{x}_0(\Omega)$ and $\tilde{x}_m(\Omega)$ are critical points, Lemma 2 shows that $\tilde{x}_1(\Omega) = x_1(\Omega)$, $\tilde{x}_2(\Omega) = x_2(\Omega)$, $\tilde{x}_0(\Omega) = x_0(\Omega)$, and $\tilde{x}_m(\Omega) = x_m(\Omega)$.

Now we can verify properties (13)...(26). In view of (51) and (53), we have $[x_1(\tilde{\Omega}), x_2(\tilde{\Omega})] \subset ((1-10^{-2})x_1(\Omega), (1+10^{-2})x_2(\Omega))$ for $\tilde{\Omega} = (1-10^{-5})\Omega$. Since $V_\Omega(x) = 10^{-5}\Omega x^{-2} + V_{\tilde{\Omega}}(x)$ and $V_{\tilde{\Omega}}(x) > 0$ outside $[x_1(\tilde{\Omega}), x_2(\tilde{\Omega})]$, we obtain

$$(55) \qquad V_\Omega(x) > 10^{-5}\Omega x^{-2} \quad \text{for} \quad x \le (1-10^{-2})x_1(\Omega)\ , \quad \text{and}$$

$$(56) \qquad V_\Omega(x) > 10^{-5}\Omega x^{-2} \quad \text{and} \quad x \ge (1+10^{-2})x_2(\Omega)\ .$$

Properties (13) and (19) with $c_1 = 10^{-2}$ are immediate from (39), (55), (56).

Similarly, $|x_0(\tilde{\Omega}) - x_0(\Omega)| < 10^{-2}x_0(\Omega)$ for $\tilde{\Omega} = (1-10^{-5})\Omega$, and we have $V'_\Omega(x) = -2\cdot 10^{-5}\Omega x^{-3} + V'_{\tilde{\Omega}}(x)$, and $V'_{\tilde{\Omega}}(x) < 0$ for $x < x_0(\tilde{\Omega})$. Hence,

$$(57) \qquad V'_\Omega(x) < -2\cdot 10^{-5}\Omega x^{-3} \quad \text{for} \quad x \le (1-10^{-2})x_0(\Omega)\ .$$

On the other hand, for all x we have

$$(58) \qquad V'_\Omega(x) = -2\Omega x^{-3} + y(x)x^{-2} - y'(x)x^{-1} > -2\Omega x^{-3}\ ,$$

since $y(x), -y'(x) > 0$.

Estimates (57), (58) yield property (20) with $c_1 = 10^{-2}$. They yield also

$$(59) \qquad 10^{-6}\Omega^{-2} \le -V'_\Omega(x) \le 10^{6}\Omega^{-2} \quad \text{for } \frac{1}{2}\Omega \le x \le \frac{3}{2}\Omega\ ,$$

since $\frac{3}{2}\Omega < (1-10^{-2})x_0(\Omega)$ by (52). Since $V_\Omega\big(x_1(\Omega)\big) = 0$ and $10^{-6}\Omega^{-2} \le S\big(x_1(\Omega)\big)\big(x_1(\Omega)\big)^{-1} \le 10^{6}\Omega^{-2}$ by (51) and $\Omega \le \varepsilon_0 \le \frac{1}{10}$, properties (14) and (15) with $c_1 = 10^{-2}$ follow from (59) and (51).

Next, we verify property (16). We distinguish three cases.

Case 1: $(1+10^{-2})x_1(\Omega) \le x \le k_1$. Then (51) implies

$$(1+10^{-3})\Omega \le x \le k_1\ .$$

We have $V_\Omega(x) = (+\Omega x^{-2} - x^{-1}) - x^{-1}\big(y(x)-1\big) < \Omega x^{-2} - x^{-1} + 10^{-50}x^{-1}$ (by (42)) $= -x^{-1}\big(1 - 10^{-50} - \Omega x^{-1}\big) < -x^{-1}\big(1 - 10^{-50} - \Omega\cdot[(1+10^{-3})\Omega]^{-1}\big) < -10^{-5}x^{-1}$. Thus,

$$V_\Omega(x) < -10^{-5} S(x) \ . \tag{60}$$

On the other hand, for all x and $\Omega > 0$ we have

$$V_\Omega(x) = \Omega x^{-2} - y(x)x^{-1} \geq -y(x)x^{-1} \geq -C\, S(x) \tag{61}$$

for a universal constant C, by Lemma 1.

Property (16) in Case 1 follows from (60) and (61).

Case 2: $k_1 \leq x \leq K_2$.

Then estimates (44) and (48) yield

$$-K_3 S(x) < V_\Omega(x) < -k_4 S(x) \ ,$$

proving property (16) in Case 2.

Case 3: $K_2 \leq x \leq (1-10^{-2})x_2(\Omega)$. Then (53) yields

$$K_2 \leq x \leq (1-10^{-3})\cdot 12\,\Omega^{-1/2} \ .$$

We have $V_\Omega(x) = \Omega x^{-2} - 144\,x^{-4} - 144\,x^{-4}\Big\{\frac{x^3 y(x)}{144} - 1\Big\} < \Omega x^{-2} - \frac{144(1-10^{-50})}{x^4}$ by (43). Thus, $-V_\Omega(x) > x^{-4}\big\{144(1-10^{-50}) - \Omega\cdot x^2\big\} > x^{-4}\big\{144(1-10^{-50}) - \Omega\cdot (1-10^{-3})^2\cdot 144\,\Omega^{-1}\big\} = 144\,x^{-4}\big\{1 - 10^{-50} - (1-10^{-3})^2\big\} > 10^{-4}x^{-4} = 10^{-4}S(x)$. Together with (61), this proves (16) in Case 3.

The proof of property (16), with $c_1 = 10^{-2}$, is complete.

Next, we verify property (22). The proof is similar to that of (16). Again we distinguish three cases.

Case 1: $(1+10^{-2})x_0(\Omega) \leq x \leq k_1$. Then (52) shows that

$$(1+10^{-3})\cdot 2\Omega \leq x \leq k_1 \ .$$

We have $V'_\Omega(x) = -2\Omega x^{-3} + x^{-2} + x^{-2}\{y(x) - 1\} - x^{-1}y'(x)$. The last two terms on the right are dominated by $10^{-50}x^{-2}$ by (42). Hence, $V'_\Omega(x) \geq -2\Omega x^{-3} + (1 - 10^{-49})x^{-2} = x^{-2}[1 - 10^{-49} - 2\Omega x^{-1}] \geq x^{-2}[1 - 10^{-49} - (1 + 10^{-3})^{-1}] > 10^{-4}x^{-2} = 10^{-4}S(x)x^{-1}$. On the other hand, for all x, $\Omega > 0$ we have

$$(62)\quad V'_\Omega(x) = -2\Omega x^{-3} + y(x)x^{-2} - y'(x)x^{-1} \leq y(x)x^{-2} - y'(x)x^{-1} < C\,S(x)x^{-1}$$

for a universal constant C, by Lemma 1.

Thus, $10^{-4}S(x)x^{-1} < V'_\Omega(x) < C\,S(x)x^{-1}$, proving property (22) in Case 1.

Case 2: $k_1 \leq x \leq K_2$.

Then (45) and (47) yield $k_5 S(x)x^{-1} < V'_\Omega(x) < K_6 S(x)x^{-1}$, which proves property (22) in Case 2.

Case 3: $K_2 \leq x \leq (1 + 10^{-2})x_2(\Omega)$.

Then (53) yields

$$K_2 \leq x \leq (1 - 10^{-3}) \cdot 12\sqrt{2}\,\Omega^{-1/2}\ .$$

We have $V'_\Omega(x) = -2\Omega x^{-3} + 4\cdot 144\, x^{-5} + 4\cdot 144\, x^{-5}\left\{\frac{x^3 y(x)}{144} - 1\right\} - 144\, x^{-4}\frac{d}{dx}\left\{\frac{x^3 y(x)}{144} - 1\right\}$. The last two terms on the right are dominated by $10^{-40}x^{-5}$, by (43). Hence

$$\begin{aligned} V'_\Omega(x) &> -2\Omega x^{-3} + (4\cdot 144 - 2\cdot 10^{-40})x^{-5} = x^{-5}\left\{4\cdot 144 - 2\cdot 10^{-40} - 2\Omega x^2\right\} \\ &\geq x^{-5}\left\{4\cdot 144 - 2\cdot 10^{-40} - 2\Omega\cdot(1 - 10^{-3})^2\cdot 2\cdot 144\,\Omega^{-1}\right\} \\ &= x^{-5}\left\{4\cdot 144 - 2\cdot 10^{-40} - 4\cdot 144\cdot(1 - 10^{-3})^2\right\} > 10^{-3}x^{-5} = 10^{-3}S(x)x^{-1}\ . \blacksquare \end{aligned}$$

This and (62) complete the proof of property (22) in Case 3.

Thus, we have verified property (22), with $c_1 = 10^{-2}$, in all cases.

Next, we verify (17) and (18). Equations (52), (53), (54) show that $[(1 - 10^{-2})x_2(\Omega), (1 + 10^{-2})x_2(\Omega)] \subset [(1 + 10^{-2})x_0(\Omega), (1 + 10^{-2})x_2(\Omega)]$. Hence, property (22) shows that

$$(63)\quad k_7 S(x)x^{-1} < V'_\Omega(x) < K_8 S(x)x^{-1}$$

$$\text{for } x \in \left[(1 - 10^{-2})x_2(\Omega), (1 + 10^{-2})x_2(\Omega)\right]\ .$$

However, $S(x)x^{-1}$ differs from $S\big(x_2(\Omega)\big)\big(x_2(\Omega)\big)^{-1}$ by at most a factor of 10, for $x \in \big[(1-10^{-2})x_2(\Omega),\ (1+10^{-2})x_2(\Omega)\big]$. Hence, (63) implies

$$(64)\quad \frac{k_7}{10} S\big(x_2(\Omega)\big)\big(x_2(\Omega)\big)^{-1} < V'_\Omega(x) < 10\, K_8 S\big(x_2(\Omega)\big)\big(x_2(\Omega)\big)^{-1} \quad \text{for } x \in \big[(1-10^{-2})x_2(\Omega), (1+10^{-2})x_2(\Omega)\big]\ .$$

Since $V_\Omega\big(x_2(\Omega)\big) = 0$, properties (17) and (18) follow easily from (64).

Next, we verify (21). Thus, suppose $x \in [(1-10^{-2})x_0(\Omega), (1+10^{-2})x_0(\Omega)]$. By (52) we have

$$(65)\qquad x \in \big[(1-2\cdot 10^{-2})\cdot 2\Omega\ ,\ (1+2\cdot 10^{-2})\cdot 2\Omega\big]\ .$$

We have also

$$(66)\qquad V''_\Omega(x) = 6\Omega x^{-4} - 2x^{-3} - 2x^{-3}\big\{y(x)-1\big\} + 2y'(x)x^{-2} - y''(x)x^{-1}\ .$$

By (42) and (49), each of the last three terms on the right is dominated by $2\cdot 10^{-50}x^{-3}$. Hence, using (65), we obtain

(67)

$$V''_\Omega(x) > 6\Omega x^{-4} - (2+10^{-40})x^{-3} > \frac{6\Omega}{(1+2\cdot 10^{-2})^4(2\Omega)^4} - \frac{(2+10^{-40})}{(1-2\cdot 10^{-2})^3(2\Omega)^3} > 10^{-2}\Omega^{-3} > 10^{-7}\cdot x^{-3} = 10^{-7}S(x)\cdot x^{-2}\ .$$

On the other hand, (66) and (42) yield also $V''_\Omega(x) \le 6\Omega x^{-4} - (2-10^{-40})x^{-3} \le 6\Omega x^{-4} \le 10^5\Omega^{-3}$ by (65). Another application of (65) gives $\Omega^{-3} < 10^7 S(x)x^{-2}$, so that

$$(68)\qquad V''_\Omega(x) < 10^{12}S(x)x^{-2}\ .$$

Property (21) is immediate from (67) and (68).

Let us verify property (23). Lemma 1 shows that $\left|\left(\frac{d}{dx}\right)^\alpha\left(\frac{y(x)}{x}\right)\right| \le C_\alpha S(x)x^{-\alpha}$ for all $\alpha \ge 0$, $x \in (0,\infty)$, with universal constants C_α. Hence, it is enough to check that $\left|\left(\frac{d}{dx}\right)^{\alpha}(\Omega x^{-2})\right| \leq C'_{\alpha} S(x) x^{-\alpha}$. This amounts to saying that $\Omega x^{-2} \leq K S(x) = K \min\{x^{-1}, x^{-4}\}$. Thus, we must show that

$$\Omega \leq Kx \quad \text{and} \quad \Omega x^2 \leq K\ , \quad \text{with } K \text{ a universal constant}\ . \tag{69}$$

However, property (23) pertains only to $x \in [(1-10^{-2})x_1(\Omega), (1+10^{-2})(x_2(\Omega))]$. Such x satisfy (69), by virtue of (51) and (53). This proves property (23).

It remains only to verify properties (24), (25), (26). These are immediate consequences of (51)...(54). The proof of Lemma 6 is complete. $\square$

Lemmas 5 and 6 produce different choices of $\hat{c}$, $\hat{C}$, c_1, C_α. To reconcile them, we use the following trivial result.

Lemma 7. *Suppose we are given positive constants c_1, $\hat{c}$, $\hat{C}$, C_α ($c_1 < 1/2$) and an interval $J \subset (0, \overline{\Omega})$. Assume that (13),...,(26) hold for $\Omega \in J$, with the given constants.*

(A) *If c'_1, $\hat{c}'$, $\hat{C}'$, C'_α are positive constants, with $c'_1 = c_1$, $\hat{c}' \leq \hat{c}$, $\hat{C}' \geq \hat{C}$, $C'_\alpha \geq C_\alpha$, then for all $\Omega \in J$, (13)...(26) hold with the new constants c'_1, $\hat{c}'$, $\hat{C}'$, C'_α.*

(B) *Given any positive c'_1 less than c_1, there exist positive constants $\hat{c}'$, $\hat{C}'$, C'_α such that for all $\Omega \in J$, (13)...(26) hold with the new constants c'_1, $\hat{c}'$, $\hat{C}'$, C'_α.*

Sketch of proof. : To verify (A), we just check that each of the properties (13)...(26) for the given c_1, $\hat{c}$, $\hat{C}$, C_α implies the corresponding property for the new constants c'_1, $\hat{c}'$, $\hat{C}'$, C'_α.

The proof of (B) is summarized in the following table.

To prove the property listed below for the new constants c_1', $\hat{c}'$, $\hat{C}'$, C_α'	we use the following properties for the old constants c_1, $\hat{c}$, $\hat{C}$, C_α.
(13)	(13), (14), (24)
(14)	(14)
(15)	(15)
(16)	(15), (16), (17)
(17)	(17)
(18)	(18)
(19)	(18), (19), (25)
(20)	(20), (21), (24)
(21)	(21)
(22)	(21), (22)
(23)	(23)
(24)	(24)
(25)	(25)
(26)	(26)

To illustrate, we work out the proofs of (16) and (13) for the new constants, which are the most complicated arguments in the above table.

The proof of (16) is divided into cases.

Case 1: Suppose $(1+c_1')x_1(\Omega) \leq x < (1+c_1)x_1(\Omega)$. Then (15) for the old constants yields

$$\hat{c}c_1' S\big(x_1(\Omega)\big) < -V_\Omega(x) < \hat{C}c_1 S\big(x_1(\Omega)\big) \ . \tag{70}$$

Also, $S(x)$ is montone decreasing and satisfies $S(Ax) \geq A^{-4}S(x)$ for $A \geq 1$. Hence,

$$(1+c_1)^{-4}S\big(x_1(\Omega)\big) \leq S(x) \leq S\big(x_1(\Omega)\big) \ , \quad \text{since we are in Case 1} \ . \tag{71}$$

From (70) and (71) we get $(\hat{c}c_1')S(x) < -V_\Omega(x) < \big(\hat{C}c_1(1+c_1)^4\big)S(x)$, which proves (16) in Case 1, provided we take $\hat{c}'$ small enough and $\hat{C}'$ large enough.

Case 2: Suppose $(1+c_1)x_1(\Omega) \le x \le (1-c_1)x_2(\Omega)$. Then (16) for the old constants implies (16) for the new constants, provided we take $\hat{c}'$ small enough and $\hat{C}'$ large enough.

Case 3: Suppose $(1-c_1)x_2(\Omega) < x \le (1-c_1')x_2(\Omega)$. Then (16) follows from the same argument used in Case 1, using (17) in place of (15).

Similarly, the proof of (13) is divided into cases.

Case 1: Suppose $0 < x \le (1-c_1)x_1(\Omega)$. Then (13) for the new constants follows from (13) for the old constants.

Case 2: Suppose $(1-c_1)x_1(\Omega) < x \le (1-c_1')x_1(\Omega)$. Then (14) gives

$$\hat{c}c_1' S\big(x_1(\Omega)\big) \le V_\Omega(x) \le \hat{C}c_1 S\big(x_1(\Omega)\big)\ . \tag{72}$$

Since $\Omega \in (0, \overline{\Omega})$, (24) shows that $\tilde{c}\Omega^{-1} < S\big(x_1(\Omega)\big) < \tilde{C}\Omega^{-1}$ with $\tilde{c}$, $\tilde{C}$ depending only on $\hat{c}$, $\hat{C}$. Hence, (72) implies $(\hat{c}, c_1'\tilde{c})\Omega^{-1} \le V_\Omega(x) \le (\hat{C}c_1\tilde{C})\Omega^{-1}$. Another application of (24) completes the proof of (13) in Case 2.

Thus, we have proven (13) and (16) for the new constants. The arguments for the remaining properties are similar or easier, and may be left to the reader. □

Combining the last three lemmas, we arrive at the following result.

Lemma 8. *Given $\varepsilon > 0$, there exist positive constants c_1, $\hat{c}$, $\hat{C}$, C_α ($c_1 < 10^{-2}$) such that (13),…,(26) hold for all $\Omega \in (0, \overline{\Omega} - \varepsilon]$.*

Proof. We may assume $\varepsilon < \varepsilon_0$, with ε_0 as in Lemma 6. Lemmas 6 and 7(B) show that for all sufficiently small c_1 there exist $\hat{c}'$, $\hat{C}'$, C_α' such that (13)…(26) hold when $\Omega \in (0, \varepsilon_0]$. Lemma 5 shows that for all sufficiently small c_1 there are $\hat{c}''$, $\hat{C}''$, C_α'' such that (13)…(26) hold when $\Omega \in [\varepsilon, \overline{\Omega} - \varepsilon]$. Taking c_1 sufficiently small, setting $\hat{c} = \min\{\hat{c}', \hat{c}''\}$, $\hat{C} = \max\{\hat{C}', \hat{C}''\}$, $C_\alpha = \max\{C_\alpha', C_\alpha''\}$, and applying Lemma 7(A), we see that (13)…(26) hold for all $\Omega \in (0, \overline{\Omega} - \varepsilon]$. □

We turn to the study of $V_\Omega(x)$ for Ω near $\overline{\Omega}$.

Lemma 9. *There exist positive constants $\overline{c}$, c_2, $\hat{c}$, $\hat{C}$, C_α such that properties (27)...(29) hold for $(1-\overline{c})\overline{\Omega} \le \Omega < \overline{\Omega}$.*

Proof. Pick $\Omega_1 < \overline{\Omega}$. For $\Omega \in [\Omega_1, \overline{\Omega})$ we have $V_\Omega \ge V_{\Omega_1}$, so that $\{x: V_\Omega(x) < 0\}$ $\subset \{x: V_{\Omega_1}(x) < 0\}$, i.e.

(73) $$x_1(\Omega_1) \le x_1(\Omega) < x_2(\Omega) \le x_2(\Omega_1)\ .$$

Recall that $x_1(\Omega) < x_0(\Omega) < x_2(\Omega)$.

Let $-\mathcal{E}(\Omega) = \min_x V_\Omega(x) = V_\Omega\big(x_0(\Omega)\big)$, and set $\hat{\Omega} = \Omega + \big(x_1(\Omega_1)\big)^2\mathcal{E}(\Omega)$. Then we have

$$V_{\hat{\Omega}}\big(x_0(\Omega)\big) = (\hat{\Omega}-\Omega)\big(x_0(\Omega)\big)^{-2} + V_\Omega\big(x_0(\Omega)\big) = \Big(\frac{x_1(\Omega_1)}{x_0(\Omega)}\Big)^2\mathcal{E}(\Omega) - \mathcal{E}(\Omega) < 0\,, \text{by (73)}\,,$$

which shows that $\min\limits_x V_{\hat{\Omega}}(x) < 0$, i.e. $\hat{\Omega} < \overline{\Omega}$. Thus,

(74) $$\overline{\Omega} - \Omega > \big(x_1(\Omega_1)\big)^2\mathcal{E}(\Omega)\ .$$

On the other hand, set $\hat{\Omega} = \Omega + \big(x_2(\Omega_1)\big)^2\mathcal{E}(\Omega)$. Then for $x \le x_2(\Omega_1)$ we have

$$V_{\hat{\Omega}}(x) = V_\Omega(x) + (\hat{\Omega} - \Omega)x^{-2} \ge -\mathcal{E}(\Omega) + \Big(\frac{x_2(\Omega_1)}{x}\Big)^2\mathcal{E}(\Omega) \ge 0\ ;$$

while for $x \ge x_2(\Omega_1)$ we have $V_{\hat{\Omega}}(x) > V_{\Omega_1}(x) \ge 0$. Thus, $V_{\hat{\Omega}}(x) \ge 0$ for all x, which shows that $\hat{\Omega} \ge \overline{\Omega}$, i.e.

(75) $$\overline{\Omega} - \Omega \le \big(x_2(\Omega_1)\big)^2\mathcal{E}(\Omega)\ .$$

If $\overline{c} > 0$ is small enough that $(1-\overline{c})\overline{\Omega} > \Omega_1$, then (74), (75) imply property (29).

Next, observe that $\big|\big(\frac{d}{dx}\big)^\alpha V_\Omega(x)\big| \le C_\alpha$ for $x \in \big[\frac{1}{2}x_1(\Omega_1), 2x_2(\Omega_1)\big]$, $\Omega \in [\Omega_1, \overline{\Omega})$. In the same region we have also $c < x < C$ and $c < S(x) < C$. Therefore, (73) yields

(76) $$\Big|\big(\frac{d}{dx}\big)^\alpha V_\Omega(x)\Big| \le C'_\alpha S(x)x^{-\alpha}$$

$$\text{for } \Omega \in [\Omega_1, \overline{\Omega}) \text{ and } x \in \big[\frac{1}{2}x_0(\Omega), 2x_0(\Omega)\big]\ .$$

Also, since $|V_\Omega'''(x)| \leq C$ for $x \in [\frac{1}{2}x_1(\Omega), 2x_2(\Omega)]$, $\Omega \in [\Omega_1, \overline{\Omega})$ by (73); and $V_\Omega''\big(x_0(\Omega)\big) > c > 0$ for $\Omega \in [\Omega_1, \overline{\Omega})$ by (8), it follows that $c' < V_\Omega''(x) < C'$ for $|x - x_0(\Omega)| < \tilde{c}$, $\Omega \in [\Omega_1, \overline{\Omega})$. Equivalently,

$$(77) \qquad \hat{c}S(x)x^{-2} < V_\Omega''(x) < \hat{C}\,S(x)x^{-2} \quad \text{for } |x - x_0(\Omega)| < \tilde{c}\ ,\ \Omega \in [\Omega_1, \overline{\Omega})\ .$$

If $|x - x_0(\Omega)| \leq c_2 x_0(\Omega)$ and $c_2 < \frac{1}{2}$ is taken small enough that (73) yields $c_2 x_0(\Omega) < c_2 x_2(\Omega_1) < \tilde{c}$, then (76) and (77) imply property (27).

It remains to check property (28). We argue as follows. For $\Omega \in [\Omega_1, \overline{\Omega})$, (12) yields

$$V_\Omega(x) \geq V_\Omega(x_0(\Omega)) + c(x - x_0\big(\Omega)\big)^2 \quad \text{for } |x - x_0(\Omega)| < c'\ .$$

Hence, (29) implies

$$(78) \qquad V_\Omega(x) \geq -C(\overline{\Omega} - \Omega) + c\big(x - x_0(\Omega)\big)^2 \quad \text{for } |x - x_0(\Omega)| < c'\ .$$

If Ω is close enough to $\overline{\Omega}$, then (78) shows that $V_\Omega(x)$ has zeros in each of the intervals $\big[x_0(\Omega) - C'(\overline{\Omega} - \Omega)^{1/2}, x_0(\Omega)\big)$, $\big(x_0(\Omega), x_0(\Omega) + C'(\overline{\Omega} - \Omega)^{1/2}\big]$. Hence,

$$|x_1(\Omega) - x_0(\Omega)|, \quad |x_2(\Omega) - x_0(\Omega)| \leq C'(\overline{\Omega} - \Omega)^{1/2} \qquad \text{for } \Omega \text{ near enough to } \overline{\Omega}\ .$$

In particular, we can find $\Omega_2 \in (\Omega_1, \overline{\Omega})$ such that

$$(79) \qquad |x_1(\Omega_2) - x_2(\Omega_2)| < c_2 x_1(\Omega_1)\ ,\ \text{with } c_2 \text{ as in (27)}\ .$$

Now let $\Omega \in (\Omega_2, \overline{\Omega})$. Then $x_0(\Omega) \in [x_1(\Omega), x_2(\Omega)] \subset [x_1(\Omega_2), x_2(\Omega_2)]$, and $|x_1(\Omega_2) - x_2(\Omega_2)| < c_2 x_0(\Omega)$, by (73) and (79). Consequently, $[x_1(\Omega_2), x_2(\Omega_2)] \subset [(1 - c_2)x_0(\Omega), (1 + c_2)x_0(\Omega)]$. It follows that $V_{\Omega_2}(x) > 0$ outside $[(1 - c_2)x_0(\Omega), (1 + c_2)x_0(\Omega)]$. Taking $\Omega_3 \in (\Omega_2, \overline{\Omega})$, we conclude that

$$V_\Omega(x) = (\Omega - \Omega_2)x^{-2} + V_{\Omega_2}(x) > (\Omega_3 - \Omega_2)x^{-2} \qquad \text{if } \Omega \in (\Omega_3, \overline{\Omega}) \text{ and } x \notin \big[(1 - c_2)x_0(\Omega), (1 + c_2)x_0(\Omega)\big]\ .$$

This implies property (28), and completes the proof of lemma 9. □

The **Main Lemma on the Thomas-Fermi Potential** follows trivially from Lemmas 8 and 9.

The Density in an Approximate Thomas-Fermi Potential

Let $V_Z^{TF}(r)$ be the Thomas-Fermi potential arising from a nucleus of charge $+Z$ fixed at the origin. Thus, $-\Delta_x V_Z^{TF}(|x|) = (\text{const})|V_Z^{TF}(|x|)|^{3/2}$ on $\mathbb{R}^3 \backslash \{0\}$, and $V_Z^{TF}(r) = -\frac{Z}{r} + O(1)$ as $r \to 0+$.

Recall that the size of $V_Z^{TF}(r)$ and its derivatives is controlled by the weight functions

$$(0) \quad S(r) = \frac{Z}{r} \quad \text{for} \quad r \leq Z^{-1/3} \ , \ S(r) = r^{-4} \quad \text{for } r \geq Z^{-1/3}$$

$$B(r) = r \quad \text{for all } r \in (0, \infty) \ .$$

Specifically, we have

(i) $\left|\left(\frac{d}{dr}\right)^\alpha V_Z^{TF}(r)\right| \leq C_\alpha S(r) r^{-\alpha} \quad (\alpha \geq 0)$,

(ii) $V_Z^{TF}(r) < -cS(r)$, and

(iii) $\frac{d}{dr} V_Z^{TF}(r) > cS(r) r^{-1}$.

It will be important to study also small perturbations of the Thomas-Fermi potential. Thus, we say that $V(r)$ is an *approximate T-F potential* if it satisfies the estimates

$$(1) \qquad \left|\left(\frac{d}{dr}\right)^\alpha V(r)\right| \leq C_\alpha S(r) r^{-\alpha} \quad (\text{all } \alpha \geq 0) \ , \quad \text{and}$$

$$(2) \qquad \left|\left(\frac{d}{dr}\right)^\alpha \{V(r) - V_Z^{TF}(r)\}\right| \leq c_0 S(r) r^{-\alpha} \quad (0 \leq \alpha \leq 2) \ ,$$

with c_0 a small enough constant, determined by the C_α in (1). In this section, we use c, C, C' etc. to denote constants determined by the C_α in (1), and by the constants ε, N, a to be introduced later. We assume that Z is large enough, depending on the C_α in (1), and on ε, N, a.

Our goal is to understand the density ρ arising from the Hamiltonian $H = -\Delta_x + V(|x|)$ for an approximate T-F potential V. By separation of variables, we are led to consider the one-dimensional densities $\rho_\ell(r)$, arising from the potentials

$$V_\ell(r) = \frac{\ell(\ell+1)}{r^2} + V(r) \ .$$

When $V = V_Z^{TF}$, the behavior of the potentials $V_\ell(r)$ is very thoroughly understood. Let us recall how $V_\ell(r)$ looks.

Let Ω be the positive root of the equation $\Omega(\Omega+1) = \max_{r>0}\big(-r^2 V(r)\big)$, and suppose the maximum is attained at $r = \check{r}$. (The sizes of these quantities are $\Omega \sim Z^{1/3}$ and $\check{r} \sim Z^{-1/3}$.) To describe $V_\ell(r)$, we distinguish between the two cases $1 \le \ell \le (1-\overline{c})\Omega$ and $(1-\overline{c})\Omega \le \ell < \Omega$ for a small, universal constant $\overline{c}$.

For $1 \le \ell \le (1-\overline{c})\Omega$, there are numbers $x_{\text{left}}(\ell) < x_0(\ell) < x_{\text{rt}}(\ell)$ with the following properties:

Regarding the size and sign of $V_\ell(r)$:

(3) In $\big(0, (1-c_1)x_{\text{left}}(\ell)\big]$ we have $V_\ell(r) \sim \frac{\ell(\ell+1)}{r^2}$.

(4) In $\big[(1-c_1)x_{\text{left}}(\ell), (1+c_1)x_{\text{left}}(\ell)\big]$ we have $|V_\ell(r)| \sim \frac{S(x_{\text{left}}(\ell))}{x_{\text{left}}(\ell)}|r - x_{\text{left}}(\ell)|$ and $V_\ell'(r) < 0$.

(5) In $[(1+c_1)x_{\text{left}}(\ell)\ ,\ (1-c_1)x_{\text{rt}}(\ell)]$ we have $V_\ell(r) \sim -S(r)$.

(6) In $[(1-c_1)x_{\text{rt}}(\ell)\ , (1+c_1)x_{\text{rt}}(\ell)]$ we have $|V_\ell(r)| \sim \frac{S(x_{\text{rt}}(\ell))}{x_{\text{rt}}(\ell)}|r - x_{\text{rt}}(\ell)|$ and $V_\ell'(r) > 0$.

(7) In $[(1+c_1)x_{\text{rt}}(\ell), \infty)$ we have $V_\ell(r) \sim \frac{\ell(\ell+1)}{r^2}$.

Regarding the derivative of $V_\ell(r)$:

(8) In $(0, (1-c_1)x_0(\ell)]$ we have $-V_\ell'(r) \sim \frac{\ell(\ell+1)}{r^3}$.

(9) In $[(1-c_1)x_0(\ell)\ ,\ (1+c_1)x_0(\ell)]$ we have $V_\ell''(r) \sim S(r)r^{-2}$ and $V_\ell'(x_0(\ell)) = 0$.

(10) In $[(1+c_1)x_0(\ell)\ ,\ (1+c_1)x_{\text{rt}}(\ell)]$ we have $V_\ell'(r) \sim S(r)r^{-1}$.

Regarding the higher derivatives of V_ℓ:

(11) In $I_\ell = \big[(1-c_1)x_{\text{left}}(\ell), (1+c_1)x_{\text{rt}}(\ell)\big]$ we have $\left|\left(\frac{d}{dr}\right)^\alpha V_\ell(r)\right| \le C_\alpha S(r) r^{-\alpha}$.

Regarding the points $x_{\text{left}}(\ell)$, $x_0(\ell)$, $x_{\text{rt}}(\ell)$:

(12) $$x_{\text{left}}(\ell)\ , x_0(\ell)\ ,\ |x_{\text{left}}(\ell) - x_0(\ell)| \sim \frac{\ell^2}{Z}$$

(13) $$x_{\text{rt}}(\ell) \sim \ell^{-1}\ .$$

Moreover,

(13a) $$x_{\text{left}}(\ell) < (1-c_1)x_0(\ell)\ , \qquad x_0(\ell) < (1-2c_1)x_{\text{rt}}(\ell)\ ,$$

(13b) $$c_1 < 1/2\ .$$

On the other hand, suppose $(1-\overline{c})\Omega \le \ell < \Omega$. Then there is a point $x_0(\ell) \sim Z^{-1/3}$ with the following properties:

(14) In $[(1-c_2)x_0(\ell), (1+c_2)x_0(\ell)]$ we have $\left|\left(\frac{d}{dr}\right)^\alpha V_\ell(r)\right| \le C_\alpha S\big(x_0(\ell)\big)\big(x_0(\ell)\big)^{-\alpha}$ and $V_\ell''(r) \sim S(r)r^{-2}$. At $r = x_0(\ell)$ we have $V_\ell' = 0$ and $-V_\ell \sim \frac{\Omega(\Omega+1)-\ell(\ell+1)}{r^2}$.

(15) Outside $[(1-c_2)x_0(\ell), (1+c_2)x_0(\ell)]$ we have $V_\ell(r) \ge \frac{c\ell(\ell+1)}{r^2}$.

Here, $0 < c_2 < 1/2$.

All these properties of $V_\ell(r) = \frac{\ell(\ell+1)}{r^2} + V(r)$ are well-known for the Thomas-Fermi potential V_Z^{TF}. (They follow by rescaling from the *Main Lemma on the T-F Potential*). Moreover, they persist under small perturbations, and therefore hold also for any approximate T-F potential.

Using the properties (3)...(15) of $V_\ell(r)$, we can verify the hypotheses of our ODE density theorems from the section "Review of Earlier Results." Specifically, we have the following results.

Lemma 1. *Set* $x_0 = \frac{\overline{C}}{Z}$, $x_{\text{crit}} = Z^{-9/10}$, $x_* = Z^{-8/10}$, $x_1 = 1/\overline{C}$, $x_{\text{big}} = \overline{C}$, $\delta = \overline{C}Z^{-3/20}$, *with* $\overline{C}$ *a large enough constant, determined by the* C_α *in (1). Then for* ℓ

$= 0$, *the potential* $V_\ell(r)$ *satisfies hypotheses* (Z0†)...(Z7†) *of the* Fourth Degenerate Density Lemma, *with the weight functions* $S(r)$ *as in (0),* $B(r) \equiv r$. *The constants in* (Z0†)...(Z7†) *depend only on the* C_α *in (1).*

Lemma 2. *Set* $x_0 = \frac{\overline{C}\ell^2}{Z}$, $x_{\text{crit}} = Z^{-9/10}$, $x_* = Z^{-8/10}$, $x_{\text{small}} = \frac{\ell^2}{\overline{C}Z}$, $x_1 = \frac{1}{\overline{C}\ell}$, $x_{\text{big}} = (1+c_1)x_{\text{rt}}(\ell)$, $\delta = \overline{C}Z^{-3/20}$, *with* $\overline{C}$ *a large enough contant, determined by the* C_α *in (1). Then for* $Z^{10^{-9}} \geq \ell \geq 1$, *the potential* $V_\ell(r)$ *satisfies hypotheses* ($\hat{Z0}$)...($\hat{Z9}$) *of the* Third Degenerate Density Lemma, *with the weight functions* $S(r)$ *as in (0),* $B(r) \equiv r$. *The constants in* ($\hat{Z0}$)...($\hat{Z9}$) *depend only on* ℓ *and on the* C_α *in (1).*

Remark. Since the constants in ($\hat{Z0}$)...($\hat{Z9}$) depend on ℓ, we can use Lemma 2 only for $1 \leq \ell \leq$ Large Constant.

Lemma 3. *Set* $I = I_\ell$ *as in (11),* $x_{\text{crit}} = Z^{-9/10}$, $E_{\text{crit}} = -Z^{18/10}$, $\delta = \overline{C}Z^{-3/20}$, *with* $\overline{C}$ *a large enough constant, determined by the* C_α *in (1). Then for* $\overline{C} \leq \ell \leq Z^{10^{-9}}$, *the potential* $V_\ell(r)$ *satisfies hypotheses* ($\overline{Z0}$)...($\overline{Z8}$) *of the* Second Degenerate Density Lemma, *with the weight functions* $S(r)$ *as in (0),* $B(r) \equiv r$. *The constants in* ($\overline{Z0}$)...($\overline{Z8}$) *depend only on the* C_α *in (1).*

Lemma 4. *Set* $I = I_\ell$ *as in (11), and take* $K = 100^{90}$, *take* $\varepsilon > 0$ *and* $N > 1$. *Let* $\hat{c}$ *be a small enough constant, depending on* ε, N *and on the* C_α *in (1).*

Then for $Z^{10^{-9}} \leq \ell \leq (1-\overline{c})\Omega$, *the potential* $V_\ell(r)$ *satisfies hypotheses (Z0)...(Z9) of the* WKB Density Theorem *in one dimension, with the weight functions* $S(r)$ *as in (0),* $B(r) \equiv r$. *The number called* Λ *in (Z0)...(Z9) is of the order of magnitude* ℓ. *The constants in (Z0)...(Z9) depend only on* ε, N, *and the* C_α *in (1).*

Lemma 5. *Suppose* $(1-\overline{c})\Omega \leq \ell < \Omega - c\Omega^{7/43}$. *Set* $\tilde{S} = \frac{\Omega(\Omega-\ell)}{\check{r}^2}$, $\tilde{B} = \frac{\check{r}(\Omega-\ell)^{1/2}}{\Omega^{1/2}}$, *and define* $I = [x_0(\ell) - h, x_0(\ell) + h]$*, with* $h = \min(c_2 x_0(\ell), \underline{C}\tilde{B})$ *and* $\underline{C}$ *a large constant determined by the* C_α *in (1). Let* $\varepsilon > 0$*,* $N > 1$ *be given. Set* $K = 100^{90}$*, and let* $\hat{c}$ *be a small enough constant, depending on* ε*,* N *and the* C_α *in (1).*

Then the potential $V_\ell(r)$*, the weight functions* $\tilde{S}$*,* $\tilde{B}$*, and the interval* I *satisfy the hypotheses (Z0)...(Z9) of the WKB Density Theorem in one dimension. The number called* Λ *in (Z0)...(Z9) is of the order of magnitude* $(\Omega - \ell)$*. The constants in (Z0)...(Z9) depend only on* ε*,* N *and the* C_α *in (1).*

Remark. The reason for using $\tilde{S}$, $\tilde{B}$, I as above is that (as we will see) $|\min V_\ell| \sim \tilde{S}$, $V_\ell'' \sim \tilde{S}\tilde{B}^{-2}$ at $x_0(\ell)$, and I is comparable to $\{V_\ell < 0\}$.

Lemma 6. *Suppose* $\Omega - c\Omega^{7/43} \le \ell < \Omega$*. Set* $x_0 = x_0(\ell)$*,* $S = S(x_0)$*,* $B = x_0$*. Let* $\varepsilon > 0$ *and* $N > 1$ *be given. Take* $K = 100^{90}$*. Then the potential* $V_\ell(r)$ *satisfies hypotheses (Z0*)...(Z6*) of the First Degenerate Density Lemma, with* $\lambda \sim S^{1/2}(\check{r})\check{r} \sim \Omega$*. The constants in (Z0*)...(Z6*) depend only on* ε*,* N *and the* C_α *in (1).*

We will use Lemma 1 for $\ell = 0$, Lemma 2 for $1 \le \ell \le$ (Large Const), Lemma 3 for (Large Const) $\le \ell \le Z^{10^{-9}}$, Lemma 4 for $Z^{10^{-9}} \le \ell \le (1 - \overline{c})\Omega$, Lemma 5 for $(1 - \overline{c})\Omega \le \ell \le \Omega - c\Omega^{7/43}$, and Lemma 6 for $\Omega - c\Omega^{7/43} \le \ell < \Omega$. Thus, all the potentials $V_\ell(r)$ $(0 \le \ell < \Omega)$ are covered by our ODE density results. For $\ell \ge \Omega$, the potential $V_\ell(r)$ is non-negative everywhere, so that $\rho_\ell(r) \equiv 0$.

We give the proofs of Lemmas 1...6.

Proof of Lemma 1.

(Z0†) is obvious from the definitions of $S(r)$, $B(r)$.

(Z1†) is immediate from (1).

(Z2†) is immediate from (ii), (iii) and (2).

(Z3†) holds, since one computes from the definitions that $\Lambda \sim \overline{C}^{1/2}$, when $\overline{C} >> 1$ and $Z > \overline{C}^{\text{power}}$.

(Z4†) follows from (1), since $x_0 = \overline{C} Z^{-1}$.

(Z5†) is proven as follows. From (ii), (iii) and (2), we see that $V(r)$ is increasing and negative on $(0, \infty)$. From the definitions we have $x_{\text{big}} < \underline{C} x_1$. From (1) we have $|V(\frac{x_1}{8})| \leq CS(\frac{x_1}{8}) \leq \underline{C} x_1^{-2}$. This proves (Z5†).

(Z6†) is immediate from (1).

(Z7†) is proven as follows. Since $V'(x) \sim S(x)x^{-1}$, we have $V(x_*) - V(x) \sim \int_x^{x_*} S(t)t^{-1}dt$ for $x \leq \frac{x_*}{2}$. Since $x_* < Z^{-1/3}$, we have $S(t) = \frac{Z}{t}$ in $[x, x_*]$, so $V(x_*) - V(x) \sim \frac{Z}{x}$ for $0 < x < \frac{1}{2}x_*$. Also for $E \in [V(x_*), 0]$ and $x < \frac{x_*}{2}$ we have $0 \leq E - V(x_*) \leq |V(x_*)| \leq CS(x_*) = C\frac{Z}{x_*} \leq C\frac{Z}{x}$. Therefore, $E - V(x) = \big(E - V(x_*)\big) + \big(V(x_*) - V(x)\big) \sim \frac{Z}{x}$ for $0 < x < \frac{1}{2}x_*$, $E \in [V(x_*), 0]$. Hence, (Z7†) follows if we show that $\int_{x_0}^{x_{\text{crit}}} \left(\frac{Z}{x}\right)^{-1/2} dx \leq c\delta \int_{x_0}^{\frac{1}{2}x_*} \left(\frac{Z}{x}\right)^{-1/2} dx$, which is immediate from the definitions. The proof of Lemma 1 is complete □

Proof of Lemma 2.

(Z$\hat{0}$) is obvious from definitions of $S(x)$, $B(x)$.

(Z$\hat{1}$) is immediate from (11), once we check that I is contained in I_ℓ. That follows from (12), (13) and the definitions of x_0, x_1.

(Z$\hat{2}$) follows from (5) and (10) once we know that $I = [x_0, x_1] \subset [(1 + c_1)x_{\text{left}}(\ell), (1 - c_1)x_{\text{rt}}(\ell)]$ and $I = [x_0, x_1] \subset [(1 + c_1)x_0(\ell), (1 + c_1)x_{\text{rt}}(\ell)]$. These inclusions follow from (12), (13) and the definitions of x_0, x_1.

(Z$\hat{3}$) holds, because one computes from the definitions that $\Lambda \sim \overline{C}^{1/2}\ell$, while the constants appearing in (Z$\hat{0}$), (Z$\hat{1}$), (Z$\hat{2}$) don't depend on $\overline{C}$, provided $\overline{C}$ is large enough.

(Z$\hat{4}$) follows from (3), since $x_{\text{small}} \leq (1 - c_1)x_{\text{left}}(\ell) < x_0$ by (12) and the definitions of x_{small}, x_0.

$(\mathrm{Z}\hat{5})$ is proven as follows. From (3), (12) and the definition of x_{small}, we have $x_{\mathrm{small}} < (1-c_1)x_{\mathrm{left}}(\ell)$ and $|V_\ell(r)| \le \frac{C\ell^2}{r^2}$ in $[x_{\mathrm{small}}, (1-c_1)x_{\mathrm{left}}(\ell)]$.

¿From (11), (12) and the definition of $S(r)$, we have $|V_\ell(r)| \le \frac{C\ell^2}{r^2}$ also in $[(1-c_1)x_{\mathrm{left}}(\ell), x_0]$. Hence in $[x_{\mathrm{small}}, x_0]$ we have $|V_\ell(r)| \le \frac{C\ell^2}{r^2} \le \frac{C'\ell^2}{x_0^2}$, which is $(\mathrm{Z}\hat{5})$ with a constant depending on ℓ.

$(\mathrm{Z}\hat{6})$ is immediate from (10), (12), (13) and the definitions of x_1, x_{big}.

$(\mathrm{Z}\hat{7})$ is proven as follows. For $r \in [\frac{x_1}{8}, (1+c_1)x_{\mathrm{rt}}(\ell)]$ we have $|V(r)| \le CS(r) = Cr^{-4} \le \frac{C'\ell^2}{x_1^2}$ by (11), (13) and the definition of x_1. This implies $(\mathrm{Z}\hat{7})$ with a constant depending on ℓ.

$(\mathrm{Z}\hat{8})$ follows from (7), since $x_{\mathrm{big}} = (1+c_1)x_{\mathrm{rt}}(\ell)$.

$(\mathrm{Z}\hat{9})$ is proven as follows. From (12), (13) and the definition of x_0, we have $(1+c_1)x_0(\ell) < x_0 < x_* < Z^{-1/3} < x_{\mathrm{rt}}(\ell)$. Hence (10) implies $V'(x) \sim S(x)x^{-1}$ in $[x_0, x_*]$.

Therefore, we may repeat the proof of $(\mathrm{Z}7^\dagger)$ in the previous lemma. The proof of Lemma 2 is complete ■

Proof of Lemma 3.

$(\mathrm{Z}\overline{0})$ is obvious from the definitions.

$(\mathrm{Z}\overline{1})$ is (11).

$(\mathrm{Z}\overline{2})$ is proven as follows. From (3)...(7) we get $\{V_\ell(r) \le 0\} = [x_{\mathrm{left}}(\ell), x_{\mathrm{rt}}(\ell)]$. From (8), (9), (10) we get $V_\ell'(r) \le 0$ on $[x_{\mathrm{left}}(\ell), x_0(\ell)]$ and $V_\ell'(r) \ge 0$ on $[x_0(\ell), x_{\mathrm{rt}}(\ell)]$. Hence $\{V_\ell(r) \le E\}$ is a non-empty subinterval of $[x_{\mathrm{left}}(\ell), x_{\mathrm{rt}}(\ell)]$ for $V_\ell(x_0(\ell)) < E \le 0$. From (0), (5) and (13a) we get $V_\ell\big(x_0(\ell)\big) \sim -\frac{Z}{x_0(\ell)}$, and thus $V_\ell\big(x_0(\ell)\big) \sim -\frac{Z^2}{\ell^2}$ by (12).

We are taking $\overline{C} \le \ell < Z^{10^{-9}}$, $E_{\mathrm{crit}} = -Z^{18/10}$, so $V_\ell\big(x_0(\ell)\big) < E \le 0$ for any $E \in [E_{\mathrm{crit}}, 0]$. Hence $E \in [E_{\mathrm{crit}}, 0]$ implies $\{V_\ell(r) \le E\} = \big[x_{\mathrm{left}}(E), x_{\mathrm{rt}}(E)\big]$, a non-empty subinterval of $[x_{\text{left}}(\ell), x_{\text{rt}}(\ell)]$. We also have $\text{dist}(x, \partial I_\ell) > cx$ for any $x \in [x_{\text{left}}(\ell), x_{\text{rt}}(\ell)]$, in particular for $x = x_{\text{left}}(E), x_{\text{rt}}(E)$. This completes the proof of $(\text{Z}\overline{2})$.

$(\text{Z}\overline{3})$ is proven as follows. If $|r - x_0(\ell)| < c_1 x_0(\ell)$, then $V_\ell(r) \sim -S(r) \sim -S(x_0(\ell))$ by (5) and (13a), and we saw that $S(x_0(\ell)) \sim \frac{Z^2}{\ell^2}$. On the other hand, $V_\ell\big(x_{\text{left}}(E)\big) = E$, and $E \in [E_{\text{crit}}, 0]$ implies $|E| << \frac{Z^2}{\ell^2}$ since $E_{\text{crit}} = -Z^{18/10}$, $\overline{C} \le \ell \le Z^{10^{-9}}$. Hence $|x_{\text{left}}(E) - x_0(\ell)| > c_1 x_0(\ell)$, and therefore $[x_{\text{left}}(E), x_{\text{left}}(E) \cdot (1 + \frac{c_1}{10})]$ does not meet $[(1 - \frac{c_1}{10})x_0(\ell), (1 + \frac{c_1}{10})x_0(\ell)]$. From (8), (9), (10) we get $|V_\ell'(r)| \ge cS(r)r^{-1}$ in $[(1 - c_1)x_{\text{left}}(\ell), (1 + c_1)x_{\text{rt}}(\ell)] \backslash [(1 - \frac{c_1}{10})x_0(\ell), (1 + \frac{c_1}{10})x_0(\ell)]$. In particular, $|V_\ell'(r)| \ge cS(r)r^{-1}$ in $[x_{\text{left}}(E), x_{\text{left}}(E) \cdot (1 + \frac{c_1}{10})]$. Since $V_\ell(x_0(\ell)) \sim -S(x_0(\ell)) < E_{\text{crit}} < E$, we have $x_0(\ell) \in \{V_\ell \le E\} = [x_{\text{left}}(E), x_{\text{rt}}(E)]$, so $x_{\text{left}}(E) \le x_0(\ell) \le x_{\text{rt}}(E)$. Therefore $x_{\text{left}}(E) \in [x_{\text{left}}(\ell), x_0(\ell)]$, so $V_\ell'(x_{\text{left}}(E)) \le 0$. So $V_\ell'(r) \le -cS(r)r^{-1}$ in $[x_{\text{left}}(E), x_{\text{left}}(E) \cdot (1 + \frac{c_1}{10})]$.
Similarly, $V_\ell'(r) \ge +cS(r)r^{-1}$ in $[(1 - \frac{c_1}{10})x_{\text{rt}}(E), x_{\text{rt}}(E)]$. This proves $(\text{Z}\overline{3})$, with c_1 replaced by $\frac{c_1}{10}$.

$(\text{Z}\overline{4})$ is proven as follows. If $x \in [(1 - c_1)x_0(\ell), (1 + c_1)x_0(\ell)]$, then $V_\ell(x) \sim -S(x) \sim -S(x_0(\ell))$, and we know that $S(x_0(\ell)) >> |E|$ for $E \in [E_{\text{crit}}, 0]$. Hence $E - V_\ell(x) \sim S(x)$. If instead $x \in [x_{\text{left}}(E) \cdot (1 + \frac{c_1}{10}), (1 - c_1)x_0(\ell)]$, then by (8) we have $-V_\ell'(r) \sim S(r)r^{-1}$ for $r \in [x_{\text{left}}(E), x]$, and therefore $E - V_\ell(x) = V_\ell(x_{\text{left}}(E)) - V_\ell(x) \sim \int_{x_{\text{left}}(E)}^{x} S(r)r^{-1}dr \ge \int_{(1 - \frac{c_1}{100})x}^{x} S(r)r^{-1}dr$ (since $x \ge x_{\text{left}}(E) \cdot (1 + \frac{c_1}{10})$) $\sim S(x)$.

Similarly, $E - V_\ell(x) \sim S(x)$ if $x \in [(1 + c_1)x_0(\ell), x_{\text{rt}}(E) \cdot (1 - \frac{c_1}{10})]$. So we know that $E - V_\ell(x) \sim S(x)$ in three intervals that cover $[(1 + \frac{c_1}{10})x_{\text{left}}(E), (1 - \frac{c_1}{10})x_{\text{rt}}(E)]$. This proves $(\text{Z}\overline{4})$, with c_1 replaced by $\frac{c_1}{10}$.

$(\text{Z}\overline{5})$ follows from (8) and (13a), which show $V_\ell'(r) < 0$ in $(0, x_{\text{left}}(\ell)]$; and from (1) and $V_\ell(r) = V(r) + \frac{\ell(\ell+1)}{r^2}$, which show that V_ℓ is C^∞.

$(\text{Z}\overline{6})$ holds, because we saw in the proof of $(\text{Z}\overline{3})$ that $x_{\text{left}}(E) \le x_0(\ell)$. Hence

$x_{\rm left}(E) < C\frac{\ell^2}{Z}$ by (12). Since $\ell \le Z^{10^{-9}}$ and $x_{\rm crit} = Z^{-9/10}$, we know that $x_{\rm left}(E) << x_{\rm crit}$ for $E \in [E_{\rm crit}, 0]$, proving $(\overline{\rm Z6})$.

$(\overline{\rm Z7})$ is proven as follows. It asserts that (for $E \in [E_{\rm crit}, 0]$)

$$\int_{x_{\rm left}(E)}^{x_{\rm crit}} \big(E - V_\ell(x)\big)_+^{-1/2} dx \le \delta \int_{x_{\rm left}(E)}^{x_{\rm rt}(E)} \big(E - V_\ell(x)\big)_+^{-1/2} dx \ .$$

We have already proven $(\overline{\rm Z3})$, $(\overline{\rm Z4})$ with c_1 replaced by $\frac{c_1}{10}$. Hence, we know that

$$\begin{aligned} E - V_\ell(x) &\sim \frac{S(x_{\rm left}(E))}{x_{\rm left}(E)} \cdot (x - x_{\rm left}(E)) \text{ for } \quad x \in [x_{\rm left}(E), (1 + \frac{c_1}{10})x_{\rm left}(E)] \\ E - V_\ell(x) &\sim S(x) \quad \text{for } x \in [x_{\rm left}(E) \cdot (1 + \frac{c_1}{10}), x_{\rm rt}(E) \cdot (1 - \frac{c_1}{10})] \\ E - V_\ell(x) &\sim \frac{S(x_{\rm rt}(E))}{x_{\rm rt}(E)} \cdot (x_{\rm rt}(E) - x) \text{ for } x \in [x_{\rm rt}(E) \cdot (1 - \frac{c_1}{10}), x_{\rm rt}(E)] \ . \end{aligned}$$

Therefore,

$$\int_{x_{\rm left}(E)}^{y} \big(E - V_\ell(x)\big)_+^{-1/2} dx \sim \int_{x_{\rm left}(E)}^{y} S^{-1/2}(x) dx$$

for $x_{\rm left}(E) \cdot (1 + \frac{c_1}{10}) \le y \le x_{\rm rt}(E)$. If also $y \le Z^{-1/3}$, then

$$\int_{x_{\rm left}(E)}^{y} S^{-1/2}(x) = \int_{x_{\rm left}(E)}^{y} \big(\frac{Z}{x}\big)^{-1/2} dx \sim Z^{-1/2} y^{3/2} \ .$$

Thus, $\int_{x_{\rm left}(E)}^{y} \big(E - V_\ell(x)\big)_+^{-1/2} dx \sim Z^{-1/2} y^{3/2}$ if $(1 + \frac{c_1}{10}) x_{\rm left}(E) < y < \min\{Z^{-1/3}, x_{\rm rt}(E)\}$. From (5), (12), (13) we have $-V_\ell(r) \sim S(r)$ for $r \in [x_0(\ell), \frac{c}{\ell}]$. Hence, $-V_\ell(r) \sim +\frac{Z}{r} >> |E_{\rm crit}| \ge |E|$ for $r \in [x_0(\ell), x_*]$, $x_* = $ (small const.) $\cdot Z^{-8/10}$. So we cannot have $x_{\rm rt}(E) \in [x_0(\ell), x_*]$. We saw in the proof of $(\overline{\rm Z3})$ that $x_{\rm rt}(E) \ge x_0(\ell)$. Therefore, $x_{\rm rt}(E) > x_*$. Consequently,

$$\int_{x_{\rm left}(E)}^{y} \big(E - V_\ell(x)\big)_+^{-1/2} dx \sim Z^{-1/2} y^{3/2} \text{if} \quad (1 + \frac{c_1}{10}) x_{\rm left}(E) < y \le x_* \ .$$

Taking $y = x_{\rm crit}$ and $y = x_*$, and recalling that $\delta = \overline{C}\, Z^{-3/20}$, we see that

$$\int_{x_{\rm left}(E)}^{x_{\rm crit}} \big(E - V_\ell(x)\big)_+^{-1/2} dx \le \delta \int_{x_{\rm left}(E)}^{x_*} \big(E - V_\ell(x)\big)_+^{-1/2} dx \ ,$$

which implies $(\overline{\rm Z7})$.

($\mathrm{Z}\overline{8}$) is immediate from the definitions and from (12), (13). In fact, $\lambda(x) = \left(\frac{Z}{x}\right)^{1/2} x = Z^{1/2}x^{1/2}$ for $x \leq Z^{-1/3}$, and $\lambda(x) = (x^{-4})^{1/2}x = x^{-1}$ for $x \geq Z^{1/3}$. Also, $x_{\text{left}}(\ell) \sim \frac{\ell^2}{Z}$ and $x_{\text{rt}}(\ell) \sim \frac{1}{\ell}$. Therefore, $\Lambda^{-1} = \int_{x_{\text{left}}(\ell)}^{Z^{-1/3}} \frac{dx}{(Z^{1/2}x^{1/2})x} + \int_{Z^{-1/3}}^{x_{\text{rt}}(\ell)} \frac{dx}{(x^{-1})x} \sim \frac{\left(x_{\text{left}}(\ell)\right)^{-1/2}}{Z^{1/2}} + x_{\text{rt}}(\ell) \sim \ell^{-1}$. Since $\ell \geq$ (Large Const.), ($\mathrm{Z}\overline{8}$) follows.

The proof of Lemma 3 is complete. ■

Proof of Lemma 4.

(Z0) is obvious from the definitions of $S(r)$, $B(r)$.

(Z1) is the estimate (11).

(Z2) and (Z5) are proven together, as follows. From (3)...(7) we get $\{V_\ell < 0\} = [x_{\text{left}}(\ell), x_{\text{rt}}(\ell)]$. By definition of I_ℓ, both $x = x_{\text{left}}(\ell)$ and $x = x_{\text{rt}}(\ell)$ satisfy $\text{dist}(x, \partial I_\ell) > c_1 x$. Hence we know (Z2) and (Z5).

(Z3) is proven as follows. With $x_0 = x_0(\ell)$, we have $V_\ell(x_0) < -cS(x_0)$ by (5), (13a); and from (9) we have $V_\ell'(x_0) = 0$ and $V_\ell'' > cS(x_0)x_0^{-2}$ in $[(1-c_1)x_0, (1+c_1)x_0]$. Hence we know (Z3).

(Z4) follows from (8), (10), since $\frac{\ell(\ell+1)}{r^3} \sim S(r)r^{-1}$ in $[x_{\text{left}}(\ell), x_0]$.

To compute Λ, recall that $\lambda(x) = \left(\frac{Z}{x}\right)^{1/2} x = Z^{1/2}x^{1/2}$ for $x \leq Z^{-1/3}$, and $\lambda(x) = (x^{-4})^{1/2}x = x^{-1}$ for $x \geq Z^{-1/3}$. Hence if $\tilde{x} \sim Z^{-1/3}$, then $\lambda(x) \sim Z^{1/2}x^{1/2}$ for $x \leq \tilde{x}$, and $\lambda(x) \sim x^{-1}$ for $x \geq \tilde{x}$. By (12), (13) we can find $\tilde{x} \sim Z^{-1/3}$ with $(1+c)x_{\text{left}}(\ell) < \tilde{x} < (1-c)x_{\text{rt}}(\ell)$. Then we have $\Lambda^{-1} \sim \int_{x_{\text{left}}(\ell)}^{\tilde{x}} \frac{dx}{(Z^{1/2}x^{1/2})x} + \int_{\tilde{x}}^{x_{\text{rt}}(\ell)} \frac{dx}{(x^{-1})x} \sim Z^{-1/2}(x_{\text{left}}(\ell))^{-1/2} + x_{\text{rt}}(\ell) \sim \ell^{-1}$. So $\Lambda \sim \ell$, as asserted in Lemma 4.

(Z5) was proven above, together with (Z2).

(Z6) is proven as follows. Since $\Lambda \sim \ell \geq Z^{10^{-9}}$, the assertion about $x \in I_{\text{BVP}} = (0, \infty)$ with $x < x_{\text{left}}(\ell) - \Lambda^K B(x_{\text{left}}(\ell))$ is vacuous, as the right-hand side is negative. For $x > x_{\text{rt}}(\ell) + \Lambda^K B(x_{\text{rt}}(\ell))$, we have $V_\ell(x) \geq \frac{c\ell^2}{x^2}$ by (7). Also, $x \sim x - x_{\text{rt}}(\ell)$ for

$x > x_{\rm rt}(\ell)+\Lambda^K B(x_{\rm rt}(\ell))$. Therefore $V_\ell(x) > \frac{c'\ell^2}{(x-x_{\rm rt}(\ell))^2}$ for $x > x_{\rm rt}(\ell)+\Lambda^k B(x_{\rm rt}(\ell))$, which implies (Z6).

(Z7) is proven as follows. For $0 < x_1 \le x_2$, we have $1 \le \frac{S(x_1)}{S(x_2)} \le \left(\frac{x_2}{x_1}\right)^4$ by definition of $S(r)$; and $1 \le \frac{B(x_2)}{B(x_1)} = \left(\frac{x_2}{x_1}\right)$. Therefore, the assertions of (Z7) follow, if the endpoints $x_{\rm left}(\ell)$, $x_{\rm rt}(\ell)$ of I satisfy $\left(\frac{x_{\rm rt}(\ell)}{x_{\rm left}(\ell)}\right)^4 < \Lambda^K$. Since $\Lambda \sim \ell$ and $K = 100^{90}$, this amounts to $\left(\frac{\ell^{-1}}{\frac{\ell^2}{Z}}\right)^4 << \ell^{(100^{90})}$, i.e. $\left(\frac{Z}{\ell^3}\right)^4 << \ell^{(100^{90})}$. That's obvious, since $\ell \ge Z^{10^{-9}}$. Thus (Z7) is proven.

(Z8) holds because we picked $\hat{c}$ small enough, depending on ε, N, C_α.

(Z9) holds because $\Lambda \sim \ell \ge Z^{10^{-9}}$ and Z is large enough. The proof of Lemma 4 is complete. ■

Proof of Lemma 5.

(Z0) is obvious, since $\tilde{S}$ and $\tilde{B}$ are constant functions.

(Z1) is proven as follows. We note first that

$$S\big(x_0(\ell)\big)\cdot\big(x_0(\ell)\big)^{-2} \sim \tilde{S}\tilde{B}^{-2} \quad \text{and that} \quad \tilde{B} \le Cx_0(\ell)\ . \tag{16}$$

In fact, since $x_0(\ell) \sim Z^{-1/3}$, we have $S\big(x_0(\ell)\big)\cdot\big(x_0(\ell)\big)^{-2} \sim Z^{4/3}\cdot(Z^{-1/3})^{-2} = Z^2$, while $\tilde{S}\tilde{B}^{-2} = \frac{\Omega^2}{\check{r}^4} \sim (Z^{1/3})^2(Z^{-1/3})^{-4} = Z^2$. Also, since $\Omega - \ell \le \bar{c}\Omega$, we have $\tilde{B} \le \bar{c}^{1/2}\check{r} \sim Z^{-1/3}$, while $x_0(\ell) \sim Z^{-1/3}$. So we know both the equations (16).

Next, note that I is contained in the interval in (14), since $h \le c_2 x_0(\ell)$. Hence in I we have from (14) that $\left|\left(\frac{d}{dr}\right)^\alpha V_\ell\right| \le C_\alpha S\big(x_0(\ell)\big)\big(x_0(\ell)\big)^{-\alpha}$. If $\alpha \ge 2$, then by (16) we have $S\big(x_0(\ell)\big)\big(x_0(\ell)\big)^{-\alpha} \le C_\alpha\tilde{S}\tilde{B}^{-\alpha}$, so

$$\left|\left(\frac{d}{dx}\right)^\alpha V_\ell\right| \le C_\alpha\tilde{S}\tilde{B}^{-\alpha} \quad \text{in} \quad I\ ,\ \text{provided}\ \alpha \ge 2\ . \tag{17}$$

Moreover at $r = x_0(\ell)$ we have from (14) that $V_\ell' = 0$ and

$$|V_\ell| \le C\frac{\Omega(\Omega+1)-\ell(\ell+1)}{\big(x_0(\ell)\big)^2} \sim \frac{\Omega(\Omega-\ell)}{\check{r}^2} = \tilde{S}\ , \tag{17bis}$$

since $x_0(\ell) \sim Z^{-1/3} \sim \check{r}$.

Since $|I| \le 2\underline{C}\tilde{B}$, Taylor's Theorem with remainder and (17) imply for $r \in I$

$$|V_\ell(r)| \le |V_\ell\big(x_0(\ell)\big)| + \underline{C}\tilde{B}|V_\ell'\big(x_0(\ell)\big)| + C\tilde{B}^2 \sup_I |V_\ell''|$$
$$\le C\tilde{S}\ , \quad \text{and}$$
$$|V_\ell'(r)| \le |V_\ell'\big(x_0(\ell)\big)| + C\tilde{B}\ \sup_I |V_\ell''| \le C\tilde{S}\tilde{B}^{-1}\ .$$

Thus, (17) holds for $\alpha = 0, 1$ also, completing the proof of (Z1).

(Z2) is proven as follows. Since I is contained in the interval in (14), we have $V_\ell'' > 0$ in I. Hence, $\{x \in I \mid V_\ell(x) < 0\}$ is a (possibly empty) subinterval. Since $x_0(\ell) \in I$ and $V_\ell\big(x_0(\ell)\big) < 0$ by (14), the subinterval is non-empty. It remains to show that the endpoints of $\{x \in I \mid V_\ell(x) < 0\}$ have distance at least $c\tilde{B}$ from the endpoints of I. That is equivalent to saying that $V_\ell(x) > 0$ if $x \in I$ and $\operatorname{dist}(x, \partial I) < c\tilde{B}$. Since we already know that $|V_\ell'| \le C\tilde{S}\tilde{B}^{-1}$ on I by (Z1) above, it is enough to show that $V_\ell > c\tilde{S}$ at the endpoints of I. We distinguish the two cases $h = c_2 x_0(\ell)$ and $h = \underline{C}\tilde{B} < c_2 x_0(\ell)$.

If $h = c_2 x_0(\ell)$, then I is the interval in (14), (15). From (15) we know that for r an endpoint of I we have $V_\ell(r) > \frac{c\ell(\ell+1)}{r^2} \sim \frac{Z^{2/3}}{(Z^{-1/3})^2} = Z^{4/3}$, while $\tilde{S} \le \frac{\Omega^2}{\check{r}^2} \sim \frac{(Z^{1/3})^2}{(Z^{-1/3})^2} = Z^{4/3}$. Hence, $V_\ell(r) > c\tilde{S}$ at the endoints of I. In the other case $h = \underline{C}\tilde{B} < c_2 x_0(\ell)$, we have from (14), (16) that $V_\ell'' \ge c\tilde{S}\tilde{B}^{-2}$ in I. Also at $x_0(\ell)$ we have $V_\ell \ge -C\tilde{S}$ by (17 bis) and $V_\ell' = 0$ by (14). The endpoints of I are $y = x_0(\ell) \pm \underline{C}\tilde{B}$, and Taylor's theorem with remainder in integral form gives

$$V_\ell(y) \ge V_\ell\big(x_0(\ell)\big) + \frac{1}{2}(\underline{C}\tilde{B})^2(c\tilde{S}\tilde{B}^{-2}) \ge -C\tilde{S} + \frac{1}{2}c\underline{C}^2\tilde{S}\ .$$

Here, C and c do not depend on $\underline{C}$. So, by taking $\underline{C}$ large enough, we get $V_\ell \ge c\tilde{S}$ at the endpoints of I.

Thus, in either case $V_\ell \ge c\tilde{S}$ at the endpoints of I. The proof of (Z2) is complete.

(Z3) is proven as follows. From (14) we have $V_\ell' = 0$ at $x_0 = x_0(\ell)$, and also from (14) we have $-V_\ell(x_0) \sim \frac{\Omega(\Omega+1)-\ell(\ell+1)}{\left(x_0(\ell)\right)^2} \sim \frac{\Omega(\Omega-\ell)}{\check{r}^2} = \tilde{S}$, since $x_0(\ell) \sim Z^{-1/3} \sim \check{r}$. To complete the proof of (Z3), we need to show that $V_\ell''(x) \geq c\tilde{S}\tilde{B}^{-2}$ for $|x-x_0| < c_3\tilde{B}$. In fact, (14) and (16) shows that $V_\ell'' \geq c\tilde{S}\tilde{B}^{-2}$ in I. (Recall that I is contained in the interval in (14), since $h \leq c_2 x_0(\ell)$.) Hence it's enough to show that $\{|x-x_0| < c_3\tilde{B}\} \subset I$, i.e. $\mathrm{dist}(x_0, \partial I) > c_0\tilde{B}$. This is immediate from $-V_\ell(x_0) \sim \tilde{S}$, which we just saw, from $|V_\ell'| \leq C\tilde{S}\tilde{B}^{-1}$ in I, which follows from (Z1) above; and from the fact that $V_\ell \geq 0$ at the endpoints of I, which follows from (Z2) above. The proof of (Z3) is complete.

(Z4) follows from the fact that $V_\ell'' \geq c\tilde{S}\tilde{B}^{-2}$ in I (as we noted above), and that $V_\ell' = 0$ at $x_0(\ell)$.

Next we compute Λ. Since $V_\ell(x_0) \sim -\tilde{S}$ and $|V_\ell'| \leq C\tilde{S}\tilde{B}^{-1}$ in I by (Z1) above, we see from (Z2) that $x_{\mathrm{rt}}(\ell) - x_{\mathrm{left}}(\ell) \geq c\tilde{B}$. On the other hand, $x_{\mathrm{rt}}(\ell) - x_{\mathrm{left}}(\ell) \leq \mathrm{diam}\, I = 2h \leq 2\underline{C}\tilde{B}$. Thus $x_{\mathrm{rt}}(\ell) - x_{\mathrm{left}}(\ell) \sim \tilde{B}$. Also, $\lambda(x) = \tilde{S}^{1/2}\tilde{B} = (\Omega - \ell)$. Therefore, $\Lambda^{-1} = \int_{x_{\mathrm{left}}(\ell)}^{x_{\mathrm{rt}}(\ell)} \frac{dx}{\lambda(x)\tilde{B}} \sim (\Omega-\ell)^{-1}$, i.e. Λ has the order of magnitude $(\Omega - \ell)$.

(Z5) is proven as follows. In view of (Z2), it is enough to show that $V_\ell > 0$ outside of I. We already know from (15) that $V_\ell > 0$ outside $J \equiv \left[x_0(\ell)(1-c_2), x_0(\ell)(1+c_2)\right]$. Inside this interval we have $V_\ell'' > c\tilde{S}\tilde{B}^{-2}$ by (14) and (16). Since $V_\ell \sim -\tilde{S}$, $V_\ell' = 0$ at $x_0(\ell)$, we conclude that

$$V_\ell(x) \geq -C\tilde{S} + \frac{1}{2}(c\tilde{S}\tilde{B}^{-2}) \cdot (\underline{C}\tilde{B})^2 \quad \text{for } x \in J, |x-x_0| \geq \underline{C}\tilde{B}\ .$$

The constants C, c here don't depend on $\underline{C}$. Hence if we pick $\underline{C}$ large enough, we get $V_\ell(x) > 0$ for $x \in J$, $|x - x_0| \geq \underline{C}\tilde{B}$. So if $x \in (0,\infty)$ satisfies $V_\ell(x) < 0$, then $x \in J$ and $|x-x_0| < \underline{C}\tilde{B}$. That is, $|x - x_0(\ell)| \leq \min(c_2 x_0(\ell), \underline{C}\tilde{B})$, i.e. $x \in I$. Thus, $V_\ell > 0$, outside I, completing the proof of (Z5).

(Z6) is proven as follows. We have $\Lambda \sim (\Omega - \ell) \geq c\Omega^{\frac{7}{43}} \sim Z^{\frac{7}{3\cdot 43}}$, while $K = 100^{90}$. Hence $\Lambda^K \geq Z^{100}$, so $\Lambda^K \tilde{B} > (1+c_2)x_0(\ell)$. This shows that $x_{\text{left}}(\ell) - \Lambda^K \tilde{B} < 0$, so the assertion of (Z6) concerning $x \in (0,\infty)$ with $x < x_{\text{left}}(\ell) - \Lambda^K \tilde{B}$ holds vacuously. Also, $x_{\text{rt}}(\ell) + \Lambda^K \tilde{B} > (1+c_2)x_0(\ell)$. Therefore, (15) shows that $V_\ell(x) > \frac{c\ell(\ell+1)}{x^2}$ for $x > x_{\text{rt}}(\ell) + \Lambda^K \tilde{B}$. We have $x - x_{\text{rt}}(\ell) \sim x$ for $x > x_{\text{rt}}(\ell) + \Lambda^K \tilde{B} > x_{\text{rt}}(\ell) + (1+c_2)x_0(\ell)$, since $x_{\text{rt}}(\ell) \in I$ and thus $x_{\text{rt}}(\ell) \leq (1+c_2)x_0(\ell)$. Therefore $V_\ell(x) > \frac{c'\ell(\ell+1)}{(x - x_{\text{rt}}(\ell))^2}$ for $x > x_{\text{rt}}(\ell) + \Lambda^K \tilde{B}$, completing the proof of (Z6).

(Z7) is trivial, since $\tilde{S}$ and $\tilde{B}$ are constant functions, and since $|I| = 2h \leq 2\underline{C}\tilde{B}$, while $\Lambda \sim (\Omega - \ell) > c\, Z^{\frac{7}{3\cdot 43}} >> \underline{C}$.

(Z8) is trivial, since we picked $\hat{c}$ to be small enough.

(Z9) is trivial, since $\Lambda \sim (\Omega - \ell) \geq c\Omega^{7/43} \sim Z^{\frac{7}{3\cdot 43}}$, and we take Z to be large enough, depending on ε, N and C_α in (1).

The proof of Lemma 5 is complete. ■

Proof of Lemma 6. Take $I = \{x \mid |x - x_0| < c_2 x_0\}$ with c_2 as in (14), (15). Thus (Z0*), (Z1*) (Z2*) are contained in (14). We have $\lambda = S^{1/2}(x_0)x_0 \sim S^{1/2}(\check{r})\check{r}$ since $x_0 \sim Z^{-1/3} \sim \check{r}$ and thus also $S(x_0) \sim S(\check{r})$. Specifically, $\lambda \sim (Z^{4/3})^{1/2} \cdot Z^{-1/3} = Z^{1/3} \sim \Omega$.

(Z3*) is proven as follows. From (14) we have $V'_\ell(x_0) = 0$, and

$$(18) \qquad -V_\ell(x_0) \sim \frac{\Omega(\Omega+1) - \ell(\ell+1)}{x_0^2} \sim \frac{\Omega(\Omega - \ell)}{x_0^2} \leq c\frac{\Omega \cdot \Omega^{\frac{7}{43}}}{x_0^2} \ .$$

On the other hand, $S^{1/2} = S^{1/2}(x_0) = \frac{\lambda}{x_0}$, so

$$(19) \qquad \lambda^{-\frac{36}{43}} S = \lambda^{-\frac{36}{43}} \cdot \frac{\lambda^2}{x_0^2} = \frac{\lambda \cdot \lambda^{\frac{7}{43}}}{x_0^2} \ .$$

Since $\lambda \sim \Omega$, we may take c small in our hypothesis $\Omega - \ell < c\Omega^{\frac{7}{43}}$, hence in (18), and obtain from (18), (19)

$$0 < -V_\ell(x_0) \leq \lambda^{-\frac{36}{43}} S \ .$$

This proves (Z3*).

(Z4*) is immediate from (15).

(Z5*) is proven as follows. Since $\lambda \sim \Omega \sim Z^{1/3}$, any $x_0 \in (0,\infty)$ satisfying $|x - x_0| > \frac{1}{2}\lambda^K B = \frac{1}{2}\lambda^K x_0$ must also satisfy $x > (1+c_2)x_0$. Hence $x \sim x - x_0$, and $V_\ell(x) \geq \frac{c\ell(\ell+1)}{x^2}$ by (15). Therefore, $V_\ell(x) > \frac{c'\ell(\ell+1)}{|x-x_0|^2}$ which implies (Z5*).

Finally (Z6*) follows from our assumption that Z is large (depending on ε, N and the C_α in (1)), since $\lambda \sim Z^{1/3}$.

The proof of Lemma 6 is complete. ■

Our plan is to use separation of variables, Lemmas 1... 6, and our density results for ODE's to control the density ρ arising from $-\Delta + V$ on $\mathbb{R}^3$. The precision of our results depends on number-theoretic properties of the potential V. Specifically, define

$$n_\ell = \int_0^\infty \left(-V_\ell(r)\right)_+^{-1/2} dr \ , \tag{20}$$

and

$$\phi_\ell = \frac{1}{\pi}\int_0^\infty \left(-V_\ell(r)\right)_+^{1/2} dr - \frac{1}{2} \ , \ \text{for } 0 \leq \ell < \Omega \ . \tag{21}$$

We will get sharper results if the ϕ_ℓ are approximately equidistributed modulo 1. Define sets $\mathcal{L}$, $\tilde{\mathcal{L}}$ by

$$\mathcal{L} = \left\{1 \leq \ell < \Omega \mid |\phi_\ell - \text{ nearest integer}| < \frac{C}{\ell}\right\} \tag{22}$$

$$\tilde{\mathcal{L}} = \left\{1 \leq \ell < \Omega \mid |\phi_\ell - \text{ nearest integer}| \ < \frac{C}{\ell^{7/43}}\right\} . \tag{23}$$

We say that the potential V has *Number-Theoretic Type* $a \geq 0$ if the following conditions hold.

$$\mathcal{D}(T) \equiv \frac{[\text{Number of } \ell \leq T \text{ belonging to } \mathcal{L}]}{T} \leq C\Omega^{-2a} \qquad \text{for} \quad \Omega^{1-4a} \leq T < \Omega \ . \tag{24}$$

$$\tilde{\mathcal{D}} \equiv \frac{[\text{number of } \ell \in \tilde{\mathcal{L}}]}{\Omega} \leq C\Omega^{-2a} \ . \tag{25}$$

Finally,

$$\Big| \sum_{\ell_1 \leq \ell \leq \ell_2} \frac{(2\ell+1)\chi_-(\phi_\ell)}{n_\ell} \Big| \leq C\Omega^{-2a} \sum_{\ell_1 \leq \ell \leq \ell_2} \frac{(2\ell+1)}{n_\ell} \tag{26}$$

$$\text{for } Z^{10^{-9}} \leq \ell_1 \leq \ell_2 < \Omega \text{ with } \ell_2 - \ell_1 \geq c\ell_2^{1-4a} \text{ and } \ell_2 \geq c\Omega^{1-4a} \ .$$

Here, $\chi_-(\cdot)$ is the elementary function appearing in our ODE density results. We expect (26) with $a > 0$ if the ϕ_ℓ are equidistributed mod 1, since χ_- is periodic and has mean value zero.

In this section, we simply assume (24), (25), (26) for an $a \geq 0$. In [FS6] [FS7], we will show that a can be taken strictly positive for the Thomas-Fermi potential V_Z^{TF}. Note that (24), (25), (26) hold trivially when $a = 0$, and that (24), (25), (26) become stronger as a increases.

We are ready to analyze the three-dimensional density ρ. Let V be an approximate T-F potential having number-theoretic type $0 \leq a < 1/43$.

Separation of variables tells us that

$$4\pi r^2 \rho(r) = \sum_{0 \leq \ell < \Omega} (2\ell+1)\rho_\ell(r) \ , \tag{27}$$

$$\text{where } \rho_\ell(\cdot) \text{ is the density arising from } -\frac{d^2}{dr^2} + V_\ell(r) \ .$$

For each ℓ, set

$$\rho_{sc}^\ell(r) = \frac{1}{\pi}\big(-V_\ell(r)\big)_+^{1/2} = \frac{1}{\pi}\big(-\frac{\ell(\ell+1)}{r^2} - V(r)\big)_+^{1/2} \tag{28}$$

$$\rho_{nt}^\ell(r) = -\Big(V_\ell(r)\Big)_+^{-1/2} \frac{\chi_-(\phi_\ell)}{n_\ell} \ , \tag{29}$$

and define $\rho_{\text{error}}^\ell(r) = \rho_\ell(r) - \{\rho_{sc}^\ell(r) + \rho_{nt}^\ell(r)\}$, so that

$$\rho_\ell(r) = \rho_{sc}^\ell(r) + \rho_{nt}^\ell(r) + \rho_{\text{error}}^\ell(r) \ . \tag{30}$$

From (27), (30) we get

(31) $$4\pi r^2\rho(r) = \rho_{\text{LOW}}(r) + \rho_{sc}(r) + \rho_{NT}(r) + \rho_{\text{ERROR}}(r) \text{ , with}$$

(32) $$\rho_{\text{LOW}}(r) = \sum_{0\le\ell<Z^{10^{-9}}} (2\ell+1)\rho_\ell(r)$$

(33) $$\rho_{sc}(r) = \sum_{Z^{10^{-9}}\le\ell<\Omega} (2\ell+1)\rho^\ell_{sc}(r)$$

(34) $$\rho_{NT}(r) = \sum_{Z^{10^{-9}}\le\ell<\Omega} (2\ell+1)\rho^\ell_{nt}(r)$$

(35) $$\rho_{\text{ERROR}}(r) = \sum_{Z^{10^{-9}}\le\ell<\Omega} (2\ell+1)\rho^\ell_{\text{error}}(r) \ .$$

Let us begin by estimating $\rho_{\text{ERROR}}(r)$. We write

(36)
$$\rho_{\text{ERROR}} = \Big[\sum_{Z^{10^{-9}}\le\ell\le(1-\overline{c})\Omega} (2\ell+1)\rho^\ell_{\text{error}}\Big] + \Big[\sum_{(1-\overline{c})\Omega<\ell\le\Omega-c\Omega^{7/43}} (2\ell+1)\rho^\ell_{\text{error}}\Big]$$
$$+ \Big[\sum_{\Omega-c\Omega^{7/43}<\ell<\Omega} (2\ell+1)\rho^\ell_{\text{error}}\Big] \equiv \rho_{\text{ERROR},1} + \rho_{\text{ERROR},2} + \rho_{\text{ERROR},3} \ .$$

For $Z^{10^{-9}} \le \ell < (1-\overline{c})\Omega$, Lemma 4 and the *WKB Density Theorem* imply the estimate

(37) $$\Big(Av_{|R-R_0|<\frac{1}{10}R_0}\Big|\int_0^R \rho^\ell_{\text{error}}(r)dr\Big|^2\Big)^{1/2}$$
$$\le Z^{-N} + C\ell^{\varepsilon-\frac{45}{43}}\int_0^{2R_0}\big(-V_\ell(r)\big)^{1/2}_+ dr + C\ell^{-1}\chi_{\ell\in\mathcal{L}}\int_0^{2R_0}\big(-V_\ell(r)\big)^{1/2}_+ \, dr \ .$$

Therefore, by definition of $\rho_{\text{ERROR},1}$, we have

(38) $$\Big(Av_{|R-R_0|<\frac{1}{10}R_0}\Big|\int_0^R \rho_{\text{ERROR},1}(r)dr\Big|^2\Big)^{1/2}$$
$$\le \sum_{Z^{10^{-9}}\le\ell\le(1-\overline{c})\Omega} (2\ell+1)\Big(Av_{|R-R_0|<\frac{1}{10}R_0}\Big|\int_0^R \rho^\ell_{\text{error}}(r)dr\Big|^2\Big)^{1/2}$$
$$\le Z^{10-N} + C\sum_{Z^{10^{-9}}\le\ell\le(1-\overline{c})\Omega} (2\ell+1)\ell^{\varepsilon-\frac{45}{43}}\int_0^{2R_0}\Big(-V_\ell(r)\Big)^{1/2}_+ dr$$
$$+ C\sum_{Z^{10^{-9}}\le\ell\le(1-\overline{c})\Omega} (2\ell+1)\ell^{-1}\int_0^{2R_0}\Big(-V_\ell(r)\Big)^{1/2}_+ dr\cdot\chi_{\ell\in\mathcal{L}}$$
$$\equiv Z^{10-N} + \text{ ERR}_1(R_0) + \text{ ERR}_2(R_0) \ .$$

Interchanging sum and integral, and recalling the definition of V_ℓ, we see that

$$\mathrm{ERR}_1(R_0) \le C\int_0^{2R_0}\Big\{\sum_{Z^{10^{-9}}\le\ell\le(1-\overline{c})\Omega}\ell^{\varepsilon-\frac{2}{43}}\big(-\frac{\ell(\ell+1)}{r^2}-V(r)\big)_+^{1/2}\Big\}dr$$

$$\le C\int_0^{2R_0}\Big\{\sum_{\substack{Z^{10^{-9}}\le\ell\le(1-\overline{c})\Omega\\ \ell(\ell+1)<-r^2V(r)}}\ell^{\varepsilon-\frac{2}{43}}\big(-V(r)\big)_+^{1/2}\Big\}dr$$

$$\le C\int_0^{2R_0}\chi_{_{-r^2V(r)>Z^{2\cdot 10^{-9}}}}\big(-r^2V(r)\big)^{\frac{\varepsilon}{2}+\frac{41}{86}}\big(-V(r)\big)^{1/2}dr$$

(39)

$$= C\int_0^{2R_0}\chi_{_{-r^2V(r)>Z^{2\cdot 10^{-9}}}}\frac{\big(-r^2V(r)\big)^{\frac{\varepsilon}{2}+\frac{42}{43}}}{r}dr\ .$$

Similarly,

$$\mathrm{ERR}_2(R_0) \le C\int_0^{2R_0}\Big\{\sum_{Z^{10^{-9}}\le\ell\le(1-\overline{c})\Omega}\chi_{\ell\in\mathcal{L}}\big(-\frac{\ell(\ell+1)}{r^2}-V(r)\big)_+^{1/2}\Big\}dr$$

$$\le C\int_0^{2R_0}\Big\{\big(-V(r)\big)_+^{1/2}\sum_{\substack{Z^{10^{-9}}\le\ell\le(1-\overline{c})\Omega\\ \ell(\ell+1)<-r^2V(r)}}\chi_{\ell\in\mathcal{L}}\Big\}dr$$

$$\le C\int_0^{2R_0}\Big\{\big(-V(r)\big)_+^{1/2}\chi_{_{-r^2V(r)>Z^{2\cdot 10^{-9}}}}\Big[\text{Number of } \ell\le\big(-r^2V(r)\big)^{1/2}\text{ belonging to }\mathcal{L}\Big]\Big\}dr$$

$$= C\int_0^{2R_0}\chi_{_{-r^2V(r)>Z^{2\cdot 10^{-9}}}}\big(-V(r)\big)_+^{1/2}\cdot\big(-r^2V(r)\big)^{1/2}\mathcal{D}\big((-r^2V(r))^{1/2}\big)dr$$

$$\le C\int_0^{2R_0}\chi_{_{Z^{2\cdot 10^{-9}}<-r^2V(r)<C\Omega^{2-8a}}}\big(-V(r)\big)_+^{1/2}\big(-r^2V(r)\big)_+^{1/2}dr$$

$$+ C\int_0^{2R_0}\chi_{_{Z^{2\cdot 10^{-9}}<-r^2V(r)}}\big(-V(r)\big)_+^{1/2}\big(-r^2V(r)\big)_+^{1/2}\cdot\Omega^{-2a}dr$$

(by (24)). That is,

$$\mathrm{ERR}_2(R_0) \le C\int_0^{2R_0}\chi_{_{Z^{2\cdot 10^{-9}}<-r^2V(r)<C\Omega^{2-8a}}}\frac{\big(-r^2V(r)\big)}{r}dr$$

(40)

$$+ C\Omega^{-2a}\int_0^{2R_0}\frac{\big(-r^2V(r)\big)}{r}\chi_{_{Z^{2\cdot 10^{-9}}<-r^2V(r)}}dr\ .$$

From (38), (39), (40), we get

$$(41)\quad \left(Av_{|R-R_0|<\frac{1}{10}R_0}\Big|\int_0^R \rho_{\mathrm{ERROR},1}(r)dr\Big|^2\right)^{1/2} \le Z^{10-N} + C\int_0^{2R_0} \chi_{_{-r^2V(r)>1}}\left(-r^2V(r)\right)_+^{\varepsilon+\frac{42}{43}}\frac{dr}{r}$$
$$+C\Omega^{-2a}\int_0^{2R_0} \chi_{_{-r^2V(r)>1}}\left(-r^2V(r)\right)_+\frac{dr}{r}+C\int_0^{2R_0} \chi_{_{-r^2V(r)<C\Omega^{2-8a}}}\left(-r^2V(r)\right)_+\frac{dr}{r}\ .$$

So we have estimated $\rho_{\mathrm{ERROR},1}$. Next we turn to $\rho_{\mathrm{ERROR},2}$.

For $(1-\overline{c})\Omega < \ell \le \Omega - c\Omega^{7/43}$, Lemma 5 and the *WKB Density Theorem* imply the estimate

$$(42)\quad \left(Av_{|R-R_0|<\frac{1}{10}R_0}\Big|\int_0^R \rho^{\ell}_{\mathrm{error}}(r)dr\Big|^2\right)^{1/2} \le Z^{-N} + C(\Omega-\ell)^{\varepsilon-\frac{45}{43}}\int_0^{2R_0}\left(-V_\ell(r)\right)_+^{1/2}dr + C(\Omega-\ell)^{-1}\chi_{_{\ell\in\tilde{\mathcal{L}}}}\int_0^{2R_0}\left(-V_\ell(r)\right)_+^{1/2}dr\ .$$

(Note that the intervals $\{|R-R_0|<\frac{1}{10}R_0\}$ and $[0,2R_0]$ in (42) are larger than their analogues in the *WKB Density Theorem*. Hence, (42) is strictly weaker than the conclusion of that Theorem.) Also from Lemma 5, we get

$$\int_0^\infty \left(-V_\ell(r)\right)_+^{1/2}dr \le C\tilde{S}^{1/2}\tilde{B} = C(\Omega-\ell)\ .$$

Moreover $\left(-V_\ell(r)\right)_+^{1/2}$ is supported in $[c\check{r},\infty)$ when $\ell > (1-\overline{c})\Omega$. Therefore

$$\int_0^{2R_0}\left(-V_\ell(r)\right)_+^{1/2}dr \le C\chi_{_{R_0>c\check{r}}}\cdot(\Omega-\ell)\ .$$

Substituting this in (42), we see that

$$\left(Av_{|R-R_0|<\frac{1}{10}R_0}\Big|\int_0^R \rho^{\ell}_{\mathrm{error}}(r)dr\Big|^2\right)^{1/2} \le Z^{-N} + C\chi_{_{R_0>c\check{r}}}(\Omega-\ell)^{\varepsilon-\frac{2}{43}} + C\chi_{_{R_0>c\check{r}}}\chi_{_{\ell\in\tilde{\mathcal{L}}}}\ .$$

Therefore, by definition of $\rho_{\mathrm{ERROR},2}$, we have the estimate

$$\begin{aligned}\left(Av_{|R-R_0|<\frac{1}{10}R_0}\left|\int_0^R \rho_{\mathrm{ERROR},2}(r)dr\right|^2\right)^{1/2} \\ \leq \sum_{(1-\overline{c})\Omega<\ell\leq\Omega-c\Omega^{7/43}} (2\ell+1)\left(Av_{|R-R_0|<\frac{1}{10}R_0}\left|\int_0^R \rho^{\ell}_{\mathrm{error}}(r)dr\right|^2\right)^{1/2} \\ \leq Z^{10-N} + C\chi_{R_0>c\check{r}}\ \Omega^{\frac{84}{43}+\varepsilon} + C\chi_{R_0>c\check{r}}\Omega^2\tilde{\mathcal{D}}\end{aligned}$$

(by definition of $\tilde{\mathcal{D}}$).

Hence, by (25), we have

$$(43)\qquad \left(Av_{|R-R_0|<\frac{1}{10}R_0}\left|\int_0^R \rho_{\mathrm{ERROR},2}(r)dr\right|^2\right)^{1/2} \leq Z^{10-N} + C\chi_{R_0>c\check{r}}\ \Omega^{2-2a}\ .$$

(Recall that $0 \leq a < 1/43$). So we have estimated $\rho_{\mathrm{ERROR},2}$. We turn to $\rho_{\mathrm{ERROR},3}$.

For $\Omega - c\Omega^{7/43} < \ell < \Omega$, Lemma 6 and the *First Degenerate Density Lemma* imply the estimate

$$\left(Av_{|R-R_0|<\frac{1}{10}R_0}\left|\int_0^R \rho^{\ell}_{\mathrm{error}}(r)dr\right|^2\right)^{1/2} \leq Z^{-N} + C\chi_{R_0>c\check{r}}\ .$$

(Here we have weakened drastically the conclusion of the *First Degenerate Density Lemma.*)

Therefore, by definition of $\rho_{\mathrm{ERROR},3}$, we have

$$\begin{aligned}(44)\quad \left(Av_{|R-R_0|<\frac{1}{10}R_0}\left|\int_0^R \rho_{\mathrm{ERROR},3}(r)dr\right|^2\right)^{1/2} \\ \leq \sum_{\Omega-c\Omega^{7/43}<\ell<\Omega} (2\ell+1)\left(Av_{|R-R_0|<\frac{1}{10}R_0}\left|\int_0^R \rho^{\ell}_{\mathrm{error}}(r)dr\right|^2\right)^{1/2} \\ \leq Z^{10-N} + C\chi_{R_0>c\check{r}} \sum_{\Omega-c\Omega^{7/43}<\ell<\Omega} (2\ell+1) \\ = Z^{10-N} + C\chi_{R_0>c\check{r}}\Omega^{50/43} < Z^{10-N} + C\chi_{R_0>c\check{r}}\Omega^{2-2a}\ ,\end{aligned}$$

again because $a \leq 1/43$.

Combining (36), (41), (43), (44), we obtain an estimate for ρ_{ERROR}, namely

$$(45)\quad \Big(Av_{|R-R_0|<\frac{1}{10}R_0}\Big|\int_0^R \rho_{\text{ERROR}}(r)dr\Big|^2\Big)^{1/2} \le Z^{10-N} + C\chi_{R_0>c\check{r}}\Omega^{2-2a} + C\int_0^{2R_0}\chi_{-r^2V(r)>1}\big(-r^2V(r)\big)_+^{\varepsilon+\frac{42}{43}}\frac{dr}{r} + C\Omega^{-2a}\int_0^{2R_0}\chi_{-r^2V(r)>1}\big(-r^2V(r)\big)_+\frac{dr}{r} + C\int_0^{2R_0}\chi_{-r^2V(r)<C\Omega^{2-8a}}\big(-r^2V(r)\big)_+\frac{dr}{r}\ .$$

We can simplify the right-hand side, because $0 \le a < 1/43$ and $\max_{r>0}\big(-r^2V(r)\big) = \Omega(\Omega+1) \sim \Omega^2$. Taking $\varepsilon > 0$ so small that $\varepsilon + \frac{42}{43} < 1-a$, we can dominate the first two integrals on the right in (45) by $C\int_0^{2R_0}\big(-r^2V(r)\big)_+^{1-a}\frac{dr}{r}$. Hence,

$$(46)\quad \Big(Av_{|R-R_0|<\frac{1}{10}R_0}\Big|\int_0^R \rho_{\text{ERROR}}(r)dr\Big|^2\Big)^{1/2} \le Z^{10-N} + C\chi_{R_0>c\check{r}}\Omega^{2-2a} + C\int_0^{2R_0}\big(-r^2V(r)\big)_+^{1-a}\frac{dr}{r} + C\int_0^{2R_0}\chi_{-r^2V(r)<C\Omega^{2-8a}}\big(-r^2V(r)\big)_+\frac{dr}{r}\ .$$

This is our basic result for ρ_{ERROR}.

Next, we study ρ_{NT}. We will use the following elementary observation.

Lemma 7. *Suppose $(u_\ell)_{0\le\ell\le\ell_2}$ is an increasing sequence of non-negative numbers. Let v_ℓ, $\tilde{v}_\ell$ be numbers that satisfy $\big|\sum_{\tilde{\ell}_1\le\ell\le\ell_2} v_\ell\big| \le \sum_{\tilde{\ell}_1\le\ell\le\ell_2}\tilde{v}_\ell$ for $0 \le \tilde{\ell}_1 \le \ell_2$. Then it follows that $\big|\sum_{0\le\ell\le\ell_2} u_\ell v_\ell\big| \le \sum_{0\le\ell\le\ell_2} u_\ell\tilde{v}_\ell$.*

Proof. The conclusion is obvious if $u_\ell = \chi_{\ell\ge\tilde{\ell}_1}$ for fixed $\tilde{\ell}_1$. The general (u_ℓ) is a linear combination of these, with non-negative coefficients. ∎

Corollary. *Suppose $(u_\ell)_{0\le\ell\le\ell_2}$ is an increasing sequence of non-negative numbers. Let v_ℓ and $v_\ell^\# > 0$ be numbers that satisfy $\big|\sum_{\ell_1\le\ell\le\ell_2} v_\ell\big| \le C\ell_2^{-2a}\sum_{\ell_1\le\ell\le\ell_2} v_\ell^\#$ for*

$\ell_1 \le \tilde{\ell}$, and $|v_\ell| \le C v_\ell^{\#}$ for all ℓ. (Here, $\tilde{\ell}$ needn't be an integer). Then

$$\Big| \sum_{0 \le \ell \le \ell_2} u_\ell v_\ell \Big| \le C \sum_{\tilde{\ell} < \ell \le \ell_2} u_\ell v_\ell^{\#} + C \ell_2^{-2a} \sum_{0 \le \ell \le \ell_2} u_\ell v_\ell^{\#} \ .$$

Proof. Take $\tilde{v}_\ell = C(\ell_2^{-2a} + \chi_{\ell > \tilde{\ell}}) v_\ell^{\#}$, and apply the preceding Lemma. ■

We use the above Corollary and inequality (26) to make the following estimate of ρ_{NT}.

Lemma 8. *For $r > 0$, let $\ell_2(r)$ be the largest integer $\ell \ge 0$ with $\ell(\ell+1) < \big(-r^2 V(r)\big)$. (If $-r^2 V(r) \le 0$, then set $\ell_2(r) \equiv 0$.) Then we have the pointwise inequality*

$$\begin{aligned} |\rho_{NT}(r)| \le C \Big[& \sum_{Z^{10^{-9}} \le \ell \le c\Omega^{1-4a}} (2\ell+1) \frac{\big(-V_\ell(r)\big)_+^{-1/2}}{n_\ell} \Big] \\ & + C \Big[\sum_{Z^{10^{-9}} \le \ell \le \ell_2(r)} (2\ell+1) \ell^{-2a} \frac{\big(-V_\ell(r)\big)_+^{-1/2}}{n_\ell} \Big] \\ & + C \Big[\sum_{\substack{\ell_2(r) - c(\ell_2(r))^{1-4a} \le \ell \le \ell_2(r) \\ \ell \ge Z^{10^{-9}}}} (2\ell+1) \frac{\big(-V_\ell(r)\big)_+^{-1/2}}{n_\ell} \Big] \\ & \equiv C\rho_{NT,1}(r) + C\rho_{NT,2}(r) + C\rho_{NT,3}(r) \ . \end{aligned}$$

Proof. Recall that $\rho_{NT}(r) = - \sum_{Z^{10^{-9}} \le \ell < \Omega} (2\ell+1) \big(-V_\ell(r)\big)_+^{-1/2} \frac{\chi_-(\phi_\ell)}{n_\ell}$. The summands are zero for $\ell > \ell_2(r)$; and also $\ell_2(r) \le \Omega$ by definition. Hence,

$$\rho_{NT}(r) = - \sum_{Z^{10^{-9}} \le \ell \le \ell_2(r)} \frac{(2\ell+1)\chi_-(\phi_\ell)}{n_\ell} \big(-V_\ell(r)\big)_+^{-1/2} \ .$$

If $\ell_2(r) \le c\Omega^{1-4a}$, then already $|\rho_{NT}(r)| \le C\rho_{NT,1}(r)$, so the conclusion of the Lemma is trivial. Hence we may assume $\ell_2(r) > c\Omega^{1-4a}$.

Set $u_\ell = \left(-V_\ell(r)\right)_+^{-1/2}\chi_{\ell\geq Z^{10^{-9}}} = \left(-\frac{\ell(\ell+1)}{r^2} - V(r)\right)^{-1/2}\chi_{\ell\geq Z^{10^{-9}}}$, $v_\ell = \chi_-(\phi_\ell)\cdot\frac{(2\ell+1)}{n_\ell}\chi_{\ell\geq Z^{10^{-9}}}$, $v_\ell^{\#} = \chi_{\ell\geq Z^{10^{-9}}}\frac{(2\ell+1)}{n_\ell}$ for $0\leq\ell\leq\ell_2(r)$. Also, set $\tilde{\ell} = \ell_2(r) - c(\ell_2(r))^{1-4a}$. Thus, u_ℓ is an increasing sequence of non-negative numbers, and $|v_\ell|\leq Cv_\ell^{\#}$. Moreover, for $\ell_1\leq\tilde{\ell}$ we have

$$\left|\sum_{\ell_1\leq\ell\leq\ell_2(r)} v_\ell\right| \leq C(\ell_2(r))^{-2a}\sum_{\ell_1\leq\ell\leq\ell_2(r)} v_\ell^{\#}\ , \quad \text{by (26)}\ . \tag{47}$$

In fact, $\ell_2(r) > c\Omega^{1-4a}$, and $\ell_2(r) - \ell_1 \geq c(\ell_2(r))^{1-4a}$, so (26) implies (47) provided $\ell_1\geq Z^{10^{-9}}$. If instead $\ell_1 < Z^{10^{-9}}$, then we can replace ℓ_1 by $\ell_1^{\min} =$ (smallest integer $\geq Z^{10^{-9}}$) without changing either the left or the right side of (47). Since $\ell_2(r) > c\Omega^{1-4a}$ and $\ell_2(r)-\ell_1^{\min} > c(\ell_2(r))^{1-4a}$, we again deduce (47) from (26). Thus, (47) is proven.

We have verified all the hypotheses in the Corollary to Lemma 7. The conclusion of that Corollary shows that $|\rho_{NT}(r)|\leq C\rho_{NT,2}(r) + C\rho_{NT,3}(r)$.

Hence the conclusion of Lemma 8 holds also when $\ell_2(r) > c\Omega^{1-4a}$. The proof of Lemma 8 is complete. ■

Let us estimate $\rho_{NT,1}(r)$. For $Z^{10^{-9}}\leq\ell\leq(1-\overline{c})\Omega$ we have

$$\int_0^R \frac{\left(-V_\ell(r)\right)_+^{-1/2}}{n_\ell}dr \leq \chi_{R>x_{\text{left}}(\ell)}\ , \tag{48}$$

by definition of n_ℓ, and by virtue of the fact that $\left(-V_\ell(r)\right)_+^{-1/2}$ is supported in $[x_{\text{left}}(\ell),\infty)$. In that range of ℓ we have also $x_{\text{rt}}(\ell) > (1+c)x_{\text{left}}(\ell)$ by (12), so

$$\chi_{R>x_{\text{left}}(\ell)} \leq C\int_0^{2R}\chi_{r\in(x_{\text{left}}(\ell),x_{\text{rt}}(\ell))}\frac{dr}{r}$$
$$= C\int_0^{2R}\chi_{\frac{\ell(\ell+1)}{r^2}+V(r)<0}\,\frac{dr}{r} = C\int_0^{2R}\chi_{-r^2V(r)>\ell(\ell+1)}\,\frac{dr}{r}\ .$$

Combining this with (48), we get

$$\int_0^R\frac{\left(-V_\ell(r)\right)_+^{-1/2}}{n_\ell}dr \leq C\int_0^{2R}\chi_{\ell(\ell+1)<-r^2V(r)}\,\frac{dr}{r}\ , \tag{49}$$
$$\text{for}\quad Z^{+10^{-9}}\leq\ell\leq(1-\overline{c})\Omega\ .$$

In particular, (49) holds for $Z^{10^{-9}} \leq \ell \leq c\Omega^{1-4a}$. Hence, by definition of $\rho_{NT,1}(r)$, we have

$$\int_0^R \rho_{NT,1}(r)dr \leq \sum_{Z^{10^{-9}} \leq \ell \leq c\Omega^{1-4a}} (2\ell+1) \cdot C \int_0^{2R} \chi_{\ell(\ell+1)<-r^2V(r)} \frac{dr}{r} \tag{50}$$

$$= C \int_0^{2R} \Big\{ \sum_{\substack{Z^{+10^{-9}} \leq \ell \leq c\Omega^{1-4a} \\ \ell(\ell+1)<-r^2V(r)}} (2\ell+1) \Big\} \frac{dr}{r} \leq C \int_0^{2R} \min\big\{ \big(-r^2V(r)\big)_+, c\Omega^{2-8a} \big\} \frac{dr}{r} \ .$$

Thus, we have estimated $\rho_{NT,1}(r)$.

Next, we estimate

$$\begin{aligned} \rho_{NT,2}(r) &= \sum_{Z^{10^{-9}} \leq \ell < \Omega} (2\ell+1)\ell^{-2a} \frac{\big(-V_\ell(r)\big)_+^{-1/2}}{n_\ell} \\ &= \Big[\sum_{Z^{10^{-9}} \leq \ell < (1-\overline{c})\Omega} (2\ell+1)\ell^{-2a} \frac{\big(-V_\ell(r)\big)_+^{-1/2}}{n_\ell} \Big] \\ &\quad + \Big[\sum_{(1-\overline{c})\Omega \leq \ell < \Omega} (2\ell+1)\ell^{-2a} \frac{\big(-V_\ell(r)\big)_+^{-1/2}}{n_\ell} \Big] \\ &\equiv \rho_{NT,2}^{\mathrm{LO}}(r) + \rho_{NT,2}^{\mathrm{HI}}(r) \ . \end{aligned} \tag{51}$$

We can estimate $\rho_{NT,2}^{\mathrm{LO}}(r)$ by the same idea as in (50). In fact, (49) yields

$$\begin{aligned} \int_0^R \rho_{NT,2}^{\mathrm{LO}}(r)dr &\leq \sum_{Z^{10^{-9}} \leq \ell < (1-\overline{c})\Omega} (2\ell+1)\ell^{-2a} \cdot C \int_0^{2R} \chi_{\ell(\ell+1)<-r^2V(r)} \frac{dr}{r} \\ &\leq C \int_0^{2R} \Big\{ \sum_{\substack{\ell(\ell+1)<-r^2V(r) \\ \ell \geq 0}} \ell^{1-2a} \Big\} \frac{dr}{r} \\ &\leq C \int_0^{2R} \big(-r^2V(r)\big)_+^{1-a} \ \frac{dr}{r} \ . \end{aligned} \tag{52}$$

To handle $\rho_{NT,2}^{\mathrm{HI}}$, we simply note that

$$\int_0^R \frac{\big(-V_\ell(r)\big)_+^{-1/2}}{n_\ell} dr \leq \chi_{R>x_{\mathrm{left}}(\ell)} \leq \chi_{R>c\check{r}} \quad \text{for} \ \ (1-\overline{c})\Omega \leq \ell < \Omega \ . \tag{53}$$

That's obvious from the definition of n_ℓ and the fact that $\left(-V_\ell(r)\right)_+^{-1/2}$ is supported in $[x_{\text{left}}(\ell), \infty)$. (See the opening paragraphs of this section for the definition of $\check{r}$.) Summing (53), we find that

$$\text{(54)} \quad \int_0^R \rho_{NT,2}^{\text{HI}}(r)dr \le \sum_{(1-\bar{c})\Omega \le \ell < \Omega} (2\ell+1)\ell^{-2a} \int_0^R \frac{\left(-V_\ell(r)\right)_+^{-1/2}}{n_\ell} dr$$
$$\le C\chi_{R>c\check{r}} \sum_{(1-\bar{c})\Omega \le \ell < \Omega} (2\ell+1)\ell^{-2a} \le C\chi_{R>c\check{r}} \Omega^{2-2a} \; .$$

Combining (51), (52), (54), we obtain

$$\text{(55)} \qquad \int_0^R \rho_{NT,2}(r)dr \le C\chi_{R>c\check{r}}\Omega^{2-2a} + C\int_0^{2R} \left(-r^2V(r)\right)_+^{1-a} \frac{dr}{r} \; .$$

Thus, we have estimated $\rho_{NT,2}$.

Next, we estimate $\rho_{NT,3}$. Define

$$\text{(56)} \qquad \rho_{\text{JUNK}}^{\ell}(r) = \frac{\left(-V_\ell(r)\right)_+^{-1/2}}{n_\ell} \chi_{\ell_2(r)-c(\ell_2(r))^{1-4a} \le \ell \le \ell_2(r)} \; ,$$

so that

$$\text{(57)} \qquad \rho_{NT,3} = \sum_{Z^{10^{-9}} \le \ell < \Omega} (2\ell+1)\rho_{\text{JUNK}}^{\ell} \; .$$

We investigate the support and integral of $\rho_{\text{JUNK}}^{\ell}$.

First suppose $Z^{10^{-9}} \le \ell \le (1-\bar{c})\Omega$. Then Lemma 4 applies, so $V_\ell(r)$ satisfies (Z0)...(Z9). In particular,

$$\text{(58)} \quad -V_\ell(r) \sim \frac{S(x_{\text{left}}(\ell))}{x_{\text{left}}(\ell)} \cdot (r - x_{\text{left}}(\ell)) \quad \text{in } J_{\text{left}} \equiv \left[x_{\text{left}}(\ell), (1+c_1)x_{\text{left}}(\ell)\right]$$

$$\text{(59)} \qquad -V_\ell(r) \sim S(r) \quad \text{in} \quad J_{\text{mid}} \equiv \left[(1+c_1)x_{\text{left}}(\ell), (1-c_1)x_{\text{rt}}(\ell)\right]$$

$$\text{(60)} \quad -V_\ell(r) \sim \frac{S(x_{\text{rt}}(\ell))}{x_{\text{rt}}(\ell)} \cdot (x_{\text{rt}}(\ell) - r) \quad \text{in } J_{\text{rt}} \equiv \left[(1-c_1)x_{\text{rt}}(\ell), x_{\text{rt}}(\ell)\right] \; ,$$

and $V_\ell(r) > 0$ outside $J_{\text{left}} \cup J_{\text{mid}} \cup J_{\text{rt}}$.

We know that $\left(-V_\ell(r)\right)_+^{-1/2}$, hence also $\rho^\ell_{\text{JUNK}}(r)$, is supported in $J_{\text{left}} \cup J_{\text{mid}} \cup J_{\text{rt}}$. In fact, $\rho^\ell_{\text{JUNK}}(r) \equiv 0$ in J_{mid}. To see this, fix $r \in J_{\text{mid}}$. By (59) we have $-V_\ell(r) > -cV(r)$, i.e. $0 > (1-c)V(r) + \frac{\ell(\ell+1)}{r^2}$, i.e. $\ell(\ell+1) < (1-c)\cdot\left(-r^2V(r)\right)$. This implies $\ell \leq (1-c')\ell_2(r)$, so that we cannot have $\ell_2(r) - c(\ell_2(r))^{1-4a} \leq \ell \leq \ell_2(r)$. (This argument uses the fact that $\ell \geq Z^{10^{-9}} >> 1$ to avoid trivial problems arising for $\ell = 0$, $-r^2V(r) << 1$. When $a = 0$, we must take care to pick c small enough in $\ell_2(r) - c(\ell_2(r))^{1-4a} \leq \ell \leq \ell_2(r)$ in order to contradict $\ell \leq (1-c')\ell_2(r)$.) Hence, the characteristic function $\chi_{\ell_2(r)-c(\ell_2(r))^{1-4a} \leq \ell \leq \ell_2(r)}$ is zero when $r \in J_{\text{mid}}$, so $\rho^\ell_{\text{JUNK}} \equiv 0$ in J_{mid}, as claimed.

Next, we study ρ^ℓ_{JUNK} in J_{left}. We need the observatioin

$$(x_{\text{left}}(\ell))^2 S(x_{\text{left}}(\ell)) \geq c\ell^2 \ . \tag{61}$$

This can be read from (12) and the definition of $S(\cdot)$, or we can invoke Lemma 4 to see that

$$c\ell \leq \Lambda \leq C\lambda(x_{\text{left}}(\ell)) = CS^{1/2}(x_{\text{left}}(\ell)) \cdot x_{\text{left}}(\ell) \ .$$

Hence we know (61). Now suppose $r \in J_{\text{left}}$ and $\ell_2(r) - c(\ell_2(r))^{1-4a} \leq \ell \leq \ell_2(r)$. Since $\ell \geq Z^{10^{-9}} >> 1$, this implies $\ell_2(r) < \ell + C\ell^{1-4a}$. Hence, $\ell_2(r) + 1 \leq \ell + C'\ell^{1-4a}$. By defintion of $\ell_2(r)$, this shows that $-r^2V(r) < (\ell + C'\ell^{1-4a})(\ell + C'\ell^{1-4a} + 1)$, which implies $-r^2V(r) < \ell(\ell+1) + C''\ell^{2-4a}$, i.e.

$$-V_\ell(r) = -V(r) - \frac{\ell(\ell+1)}{r^2} < C''\frac{\ell^{2-4a}}{r^2} \ , \quad \text{whenever } r \in J_{\text{left}} \text{ and } \ell_2(r) - c(\ell_2(r))^{1-4a} \leq \ell \leq \ell_2(r) \ . \tag{62}$$

From (61) we see that $\frac{\ell^2}{r^2} < CS(x_{\text{left}}(\ell))$ for $r \in J_{\text{left}}$.

Therefore, (62) implies

$$-V_\ell(r) < C''\ell^{-4a}S(x_{\text{left}}(\ell)) \ ,$$

$$\text{whenever } r \in J_{\text{left}} \text{ and } \ell_2(r) - c(\ell_2(r))^{1-4a} \leq \ell \leq \ell_2(r) \ .$$

In view of (58), this means that $r \in J_{\text{left}}$ and $\ell_2(r) - c(\ell_2(r))^{1-4a} \leq \ell \leq \ell_2(r)$ imply $r \in [x_{\text{left}}(\ell), (1 + C\ell^{-4a})x_{\text{left}}(\ell)]$.

Hence

$$(63) \qquad (\text{supp } \rho^{\ell}_{\text{JUNK}}) \cap J_{\text{left}} \subset [x_{\text{left}}(\ell), (1 + C\ell^{-4a})x_{\text{left}}(\ell)] \ .$$

Similarly,

$$(64) \qquad (\text{supp } \rho^{\ell}_{\text{JUNK}}) \cap J_{\text{rt}} \subset [(1 - C\ell^{-4a})x_{\text{rt}}(\ell), x_{\text{rt}}(\ell)] \ .$$

From (58), (63) and the definition (56) of $\rho^{\ell}_{\text{JUNK}}$, we have

$$(65) \quad \rho^{\ell}_{\text{JUNK}} \leq \frac{C}{n_\ell}\Big[\frac{S(x_{\text{left}}(\ell))}{x_{\text{left}}(\ell)} \cdot (r - x_{\text{left}}(\ell))\Big]^{-1/2} \chi_{r \in [x_{\text{left}}(\ell), (1+C\ell^{-4a})x_{\text{left}}(\ell)]} \qquad \text{for} \quad r \in J_{\text{left}} \ .$$

A similar estimate holds in J_{rt}.

From (58) and the definition of n_ℓ, we get the lower bound

$$\begin{aligned} n_\ell = \int_0^\infty \big(-V_\ell(r)\big)_+^{-1/2} dr &\geq c \int_{J_{\text{left}}} \Big[\frac{S(x_{\text{left}}(\ell))}{x_{\text{left}}(\ell)}(r - x_{\text{left}}(\ell))\Big]^{-1/2} dr \\ &\geq c' S^{-1/2}(x_{\text{left}}(\ell)) \cdot x_{\text{left}}(\ell) \ . \end{aligned}$$

This and (65) yield

$$\int_{J_{\text{left}}} \rho^{\ell}_{\text{JUNK}}(r)dr \leq C\ell^{-2a} \ .$$

A similar estimate holds for J_{rt}, and we know that $\rho^{\ell}_{\text{JUNK}}$ is supported in $J_{\text{left}} \cup J_{\text{rt}}$. Therefore, $\int_0^\infty \rho^{\ell}_{\text{JUNK}}(r)dr \leq C\ell^{-2a}$. Again using $\text{supp}(\rho^{\ell}_{\text{JUNK}}) \subset J_{\text{left}} \cup J_{\text{rt}} \subset [x_{\text{left}}(\ell), \infty)$, we obtain

$$(66) \qquad \int_0^R \rho^{\ell}_{\text{JUNK}}(r)dr \leq C\ell^{-2a}\chi_{R \in [x_{\text{left}}(\ell), \infty)} \quad \text{for } Z^{10^{-9}} \leq \ell \leq (1 - \overline{c})\Omega \ .$$

For $Z^{10^{-9}} \leq \ell \leq (1 - \overline{c})\Omega$ we have $x_{\text{rt}}(\ell) > (1 + c)x_{\text{left}}(\ell)$, so $\int_0^{2R} \chi_{V_\ell(r)<0} \frac{dr}{r} = \int_0^{2R} \chi_{\frac{\ell(\ell+1)}{r^2} + V(r) < 0} \frac{dr}{r} \geq c\chi_{R \in [x_{\text{left}}(\ell), \infty)}$. Hence (66) implies

$$(67) \quad \int_0^R \rho^{\ell}_{\text{JUNK}}(r) \leq C\ell^{-2a} \int_0^{2R} \chi_{\frac{\ell(\ell+1)}{r^2} + V(r) < 0} \frac{dr}{r} \qquad \text{for} \quad Z^{10^{-9}} \leq \ell \leq (1 - \overline{c})\Omega \ .$$

This is our basic estimate for $\rho^\ell_{\rm JUNK}$ when $Z^{10^{-9}} \leq \ell \leq (1-\overline{c})\Omega$.

Next we derive an analogue of (67) for $(1-\overline{c})\Omega \leq \ell \leq \Omega - c'\Omega^{1-4a}$. Here, c' is a small constant to be fixed after a few paragraphs. Fix ℓ in this range, and apply Lemma 5. Thus we have

$$-V_\ell(r) \sim \frac{\tilde{S}}{\tilde{B}}(r - x_{\rm left}(\ell)) \quad \text{in } J_{\rm left} \equiv [x_{\rm left}(\ell), x_{\rm left}(\ell) + c_1\tilde{B}] \tag{68}$$

$$-V_\ell(r) \sim \tilde{S} \quad \text{in } J_{\rm mid} \equiv [x_{\rm left}(\ell) + c_1\tilde{B}, x_{\rm rt}(\ell) - c_1\tilde{B}] \tag{69}$$

$$-V_\ell(r) \sim \frac{\tilde{S}}{\tilde{B}}(x_{\rm rt}(\ell) - r) \quad \text{in } J_{\rm rt} \equiv [x_{\rm rt}(\ell) - c_1\tilde{B}, x_{\rm rt}(\ell)] \tag{70}$$

and $V_\ell(r) > 0$ outside $J_{\rm left} \cup J_{\rm mid} \cup J_{\rm rt}$.

Here, $\tilde{S} = \frac{\Omega(\Omega-\ell)}{\check{r}^2}$; $|J_{\rm left}|$, $|J_{\rm rt}|$, $|J_{\rm mid}| \sim \tilde{B}$; and

$$r \sim \check{r} \quad \text{for } r \in J_{\rm left} \cup J_{\rm mid} \cup J_{\rm rt}\ . \tag{71}$$

Therefore,

$$n_\ell = \int_0^\infty \left(-V_\ell(r)\right)_+^{-1/2} dr \sim \tilde{S}^{-1/2}\tilde{B}\ . \tag{72}$$

Note that $\left(-V_\ell(r)\right)_+^{-1/2}$, hence also $\rho^\ell_{\rm JUNK}(r)$, is supported in $J_{\rm left} \cup J_{\rm mid} \cup J_{\rm rt}$. Suppose $r \in J_{\rm left} \cup J_{\rm mid} \cup J_{\rm rt}$ belongs to the support of $\rho^\ell_{\rm JUNK}$. Then $\ell_2(r) - c(\ell_2(r))^{1-4a} \leq \ell \leq \ell_2(r)$ with a small constant c. Since $(1-\overline{c})\Omega \leq \ell < \Omega$, this implies $\ell_2(r) \leq \ell + 2c\Omega^{1-4a}$, hence $\ell_2(r) + 1 \leq \ell + 3c\Omega^{1-4a}$. By definition of $\ell_2(r)$, this yields

$$-r^2 V(r) \leq (\ell + 3c\Omega^{1-4a})(\ell + 3c\Omega^{1-4a} + 1) \leq \ell(\ell+1) + 10\, c\Omega^{2-4a}\ .$$

Therefore

$$-V_\ell(r) = -V(r) - \frac{\ell(\ell+1)}{r^2} < \frac{10\, c\Omega^{2-4a}}{r^2} \quad \text{for } r \in \text{ supp } \rho^\ell_{\rm JUNK}\ . \tag{73}$$

If $r \in J_{\text{mid}}$, then (69) and (73) show that $\tilde{S} < \frac{\tilde{c}\Omega^{2-4a}}{r^2}$. We can make $\tilde{c}$ small by taking c small. From (71) and the definition of $\tilde{S}$, we conclude that

$$(\Omega - \ell) \le \tilde{c}'\Omega^{1-4a} \; . \tag{74}$$

On the other hand, we are studying ℓ in the range $(1-\overline{c})\Omega \le \ell \le \Omega - c'\Omega^{1-4a}$. This contradicts (74), provided we take c small enough in (56) and pick $c' = 2\tilde{c}'$. Therefore, no $r \in J_{\text{mid}}$ can belong to the support of $\rho^{\ell}_{\text{JUNK}}$. Now we know that supp $\rho^{\ell}_{\text{JUNK}} \subset J_{\text{left}} \cup J_{\text{rt}}$.

Suppose $r \in (\text{supp } \rho^{\ell}_{\text{JUNK}}) \cap J_{\text{left}}$. ¿From (68) and (73) we get

$$\frac{\tilde{S}}{\tilde{B}}(r - x_{\text{left}}(\ell)) \le C\frac{\Omega^{2-4a}}{r^2} \le C'\frac{\Omega^{2-4a}}{\check{r}^2} \qquad \text{(by (71))}.$$

By definition of $\tilde{S}$, this is equivalent to $\frac{(\Omega-\ell)}{\tilde{B}}(r - x_{\text{left}}(\ell)) \le C'\Omega^{1-4a}$, i.e.

$$r \le x_{\text{left}}(\ell) + \frac{C'\Omega^{1-4a}}{\Omega - \ell}\tilde{B} \quad \text{for } r \in J_{\text{left}} \cap \text{ supp } \rho^{\ell}_{\text{JUNK}} \; . \tag{75}$$

Putting (68), (72), (75) into the definition of $\rho^{\ell}_{\text{JUNK}}$, we obtain the inequality

$$\rho^{\ell}_{\text{JUNK}}(r) \le C\chi_{{}_{0<r-x_{\text{left}}(\ell)<\frac{C'\Omega^{1-4a}}{\Omega-\ell}\tilde{B}}}(\tilde{S}^{-1/2}\tilde{B})^{-1}\Big[\frac{\tilde{S}}{\tilde{B}}(r - x_{\text{left}}(\ell))\Big]^{-1/2} \qquad \text{for } r \in J_{\text{left}} \; .$$

Hence,

$$\int_{J_{\text{left}}} \rho^{\ell}_{\text{JUNK}}(r)dr \le C\Big(\frac{\Omega^{1-4a}}{\Omega - \ell}\Big)^{1/2} \; .$$

A similar inequality holds for J_{rt}. Since $\rho^{\ell}_{\text{JUNK}}$ is supported in $J_{\text{left}} \cup J_{\text{rt}} \subset [c\check{r}, \infty)$, it follows that

$$\int_0^R \rho^{\ell}_{\text{JUNK}}(r)dr \le C\chi_{R>c\check{r}}\Big(\frac{\Omega^{1-4a}}{\Omega - \ell}\Big)^{1/2} \,, \qquad \text{for } (1-\overline{c})\Omega \le \ell \le \Omega - c'\Omega^{1-4a} \; . \tag{76}$$

This is our basic estimate for $\rho^{\ell}_{\text{JUNK}}$ when $(1-\overline{c})\Omega < \ell \le \Omega - c'\Omega^{1-4a}$.

For $\Omega - c'\Omega^{1-4a} < \ell < \Omega$, we use the obvious inequality $\int_0^R \rho^\ell_{\text{JUNK}}(r)dr \le \int_0^\infty \frac{\left(-V_\ell(r)\right)_+^{-1/2}}{n_\ell}dr = 1$ (any ℓ). Since supp $\rho^\ell_{\text{JUNK}} \subset$ supp$(V_\ell(r))_+^{-1/2} \subset [c\check{r}, \infty)$ for the ℓ in question, it follows that

$$\int_0^R \rho^\ell_{\text{JUNK}}(r)dr \le \chi_{R>c\check{r}} \quad \text{for } \Omega - c'\Omega^{1-4a} < \ell < \Omega \, . \tag{77}$$

We can now control $\rho_{NT,3}(r)$ by using (57), (67), (76), (77). ¿From (57) we get

$$\rho_{NT,3}(r) = \rho_{\text{JUNK},1}(r) + \rho_{\text{JUNK},2}(r) + \rho_{\text{JUNK},3}(r) \quad \text{with} \tag{78}$$

$$\rho_{\text{JUNK},1}(r) = \sum_{Z^{10^{-9}} \le \ell \le (1-\overline{c})\Omega} (2\ell+1)\rho^\ell_{\text{JUNK}}(r) \tag{79}$$

$$\rho_{\text{JUNK},2}(r) = \sum_{(1-\overline{c})\Omega < \ell \le \Omega - c'\Omega^{1-4a}} (2\ell+1)\rho^\ell_{\text{JUNK}}(r) \tag{80}$$

$$\rho_{\text{JUNK},3}(r) = \sum_{\Omega - c'\Omega^{1-4a} < \ell < \Omega} (2\ell+1)\rho^\ell_{\text{JUNK}}(r) \, . \tag{81}$$

Equations (67) and (79) yield

$$\begin{aligned} \int_0^R \rho_{\text{JUNK},1}(r)dr &\le C \sum_{Z^{10^{-9}} \le \ell \le (1-\overline{c})\Omega} (2\ell+1) \int_0^{2R} \ell^{-2a} \chi_{\frac{\ell(\ell+1)}{r^2} + V(r) < 0} \frac{dr}{r} \\ &\le C' \int_0^{2R} \Big\{ \sum_{Z^{10^{-9}} \le \ell \le (1-\overline{c})\Omega} \ell^{1-2a} \chi_{\ell < (-r^2 V(r))_+^{1/2}} \Big\} \frac{dr}{r} \\ &\le C'' \int_0^{2R} \left(-r^2 V(r)\right)_+^{1-a} \frac{dr}{r} \end{aligned} \tag{82}$$

Equations (76) and (80) yield

$$\begin{aligned} \int_0^R \rho_{\text{JUNK},2}(r)dr &= \sum_{(1-\overline{c})\Omega < \ell \le \Omega - c'\Omega^{1-4a}} (2\ell+1) \int_0^R \rho^\ell_{\text{JUNK}}(r)dr \\ &\le C\chi_{R>c\check{r}} \sum_{(1-\overline{c})\Omega < \ell \le \Omega - c'\Omega^{1-4a}} (2\ell+1) \Big(\frac{\Omega^{1-4a}}{\Omega - \ell}\Big)^{1/2} \le C'\chi_{R>c\check{r}} \Omega^{2-2a} \, . \end{aligned} \tag{83}$$

Equations (77) and (81) yield

$$\int_0^R \rho_{\text{JUNK},3}(r)dr = \sum_{\Omega - c'\Omega^{1-4a} < \ell < \Omega} (2\ell+1) \int_0^R \rho^{\ell}_{\text{JUNK}}(r)dr \tag{84}$$
$$\leq \sum_{\Omega - c'\Omega^{1-4a} < \ell < \Omega} (2\ell+1)\chi_{R>c\check{r}} \leq C\Omega^{2-4a}\chi_{R>c\check{r}} \leq C\chi_{R>c\check{r}}\Omega^{2-2a} \ .$$

Combining (78) with (82), (83), (84), we obtain

$$\int_0^R \rho_{NT,3}(r)dr \leq C\chi_{R>c\check{r}}\Omega^{2-2a} + C\int_0^{2R} \left(-r^2V(r)\right)_+^{1-a}\frac{dr}{r} \ . \tag{85}$$

At last we can estimate ρ_{NT}. In fact, Lemma 8 and estimates (50), (55) and (85) together tell us that

$$\left|\int_0^R \rho_{NT}(r)dr\right| \leq C\chi_{R>c\check{r}}\Omega^{2-2a} + C\int_0^{2R} \left(-r^2V(r)\right)_+^{1-a}\frac{dr}{r} \tag{86}$$
$$+ C\int_0^{2R} \min\left\{(-r^2V(r))_+, c\Omega^{2-8a}\right\}\frac{dr}{r} \ .$$

This is our basic result for ρ_{NT}.

Let us review what has happened so far. Equation (31) expresses the density $\rho(r)$ in terms of ρ_{LOW}, ρ_{sc}, ρ_{NT}, ρ_{ERROR}, which are defined by (32)...(35). We have estimated ρ_{ERROR} and ρ_{NT} by (46) and (86). It remains to understand ρ_{sc} and estimate ρ_{LOW}.

Next we study ρ_{sc}, which is of course the main term in ρ. We will prove the following elementary result, from which the behavior of ρ_{sc} can be read off easily.

Lemma 9. *For all real numbers W, we have*

$$\sum_{\ell \geq Z^{10^{-9}}} (2\ell+1)\left(W - \ell(\ell+1)\right)_+^{1/2} = \frac{2}{3}W^{3/2}\chi_{W>Z^{2\cdot 10^{-9}}}$$
$$+ O\left(Z^{2\cdot 10^{-9}}W^{1/2}\chi_{W>Z^{2\cdot 10^{-9}}} + W^{3/4}\chi_{W>Z^{2\cdot 10^{-9}}}\right) \ .$$

Proof. If $W \leq 2Z^{2\cdot 10^{-9}}$, then the conclusion of the Lemma is trivial. Suppose $W > 2Z^{2\cdot 10^{-9}}$.

Let $t_{\max}$ be the positive root of $t(t+1) = W$, and set

$$G(t) = \big(W - t(t+1)\big)^{1/2} \quad \text{for } Z^{10^{-9}} \le t \le t_{\max} \ .$$

We will bound the derivatives of $G(t)$. In fact, $\big(\frac{d}{dt}\big)^m G(t)$ is a sum of terms of the form

$$\text{(87)} \quad \big(W - t(t+1)\big)^{\frac{1}{2}-A} \cdot \prod_{\nu=1}^{A} \big(\frac{d}{dt}\big)^{m_\nu} \{t(t+1)\} \ , \qquad \text{with } m_\nu \ge 1 \text{ and } m_1 + \ldots + m_A = m \ .$$

For a nonzero term we must have $m_\nu \le 2$, so $1 \le m_\nu \le 2$ and $A \le m_1 + \ldots + m_A \le 2A$. Thus $A \le m \le 2A$, i.e. $\frac{m}{2} \le A \le m$. Since $\big|\big(\frac{d}{dt}\big)^{m_\nu} \{t(t+1)\}\big| \le Ct^{2-m_\nu}$ for $t \ge Z^{10^{-9}}$, the term (87) is dominated by $\big(W - t(t+1)\big)^{\frac{1}{2}-A} t^{2A-m}$. Therefore,

$$\begin{aligned} \Big|\big(\frac{d}{dt}\big)^m G(t)\Big| &\le C_m \sum_{\frac{m}{2} \le A \le m} \big(W - t(t+1)\big)^{\frac{1}{2}-A} \ t^{2A-m} \\ \text{(88)} \qquad &= C_m \sum_{\frac{m}{2} \le A \le m} \big(W - t(t+1)\big)^{1/2} t^{-m} \cdot \big(\frac{t^2}{W - t(t+1)}\big)^A \ . \end{aligned}$$

We distinguish the cases $t \le \frac{1}{2} t_{\max}$, $t > \frac{1}{2} t_{\max}$. If $t \le \frac{1}{2} t_{\max}$, then $\frac{t^2}{W - t(t+1)} \le C$, so the largest term on the right of (88) comes from $A = \frac{m}{2}$. Hence

$$\text{(89)} \quad \big|\big(\frac{d}{dt}\big)^m G(t)\big| \le C'_m \big(W - t(t+1)\big)^{\frac{1}{2}-\frac{m}{2}} \le C''_m W^{\frac{1}{2}-\frac{m}{2}} \qquad \text{if} \quad Z^{10^{-9}} \le t \le \frac{1}{2} t_{\max} \ .$$

If $t_{\max} \ge t \ge \frac{1}{2} t_{\max}$, then

$$\text{(90)} \qquad \big[W - t(t+1)\big] \sim W^{1/2}(t_{\max} - t) \ .$$

Therefore, $\frac{t^2}{W - t(t+1)} \sim \frac{W}{W^{1/2}(t_{\max} - t)} > c$, so the largest term in (88) comes from $A = m$. Thus, (88) and (90) yield

$$\begin{aligned} \big|\big(\frac{d}{dt}\big)^m G(t)\big| &\le C'_m \big[W^{1/2}(t_{\max} - t)\big]^{\frac{1}{2}-m} [W^{1/2}]^m \\ \text{(91)} \qquad &= C'_m \big[W^{1/2}(t_{\max} - t)\big]^{1/2} \cdot (t_{\max} - t)^{-m} \ , \end{aligned}$$

for $\frac{1}{2}t_{\max} \leq t < t_{\max}$.

From (89) and (91) we see that

$$(92)\quad \Big|\Big(\frac{d}{dt}\Big)^m G(t)\Big| \leq C_m \big[W^{1/2}(t_{\max}-t)\big]^{1/2} \cdot (t_{\max}-t)^{-m} \qquad \text{for} \quad Z^{10^{-9}} \leq t < t_{\max}\ .$$

Now set $F(t) = (2t+1)\cdot\big(W - t(t+1)\big)^{1/2} = (2t+1)G(t)$ for $Z^{10^{-9}} \leq t < t_{\max}$. Since

$$\Big(\frac{d}{dt}\Big)^m F(t) = (2t+1)\Big(\frac{d}{dt}\Big)^m G(t) + (\mathrm{const}_m)\Big(\frac{d}{dt}\Big)^{m-1} G(t) \quad \text{for} \quad m \geq 1\ ,$$

estimate (92) implies

$$(93)\qquad \Big|\Big(\frac{d}{dt}\Big)^m F(t)\Big| \leq C_m \sigma(t)\tau^{-m}(t)\ , \quad \text{with}$$

$$(94)\quad \sigma(t) = W^{1/4} t (t_{\max}-t)^{1/2} \quad \text{and} \quad \tau(t) = \min\{t, t_{\max}-t\} \qquad \text{for} \quad Z^{10^{-9}} \leq t < t_{\max}. \qquad (\text{Recall } t_{\max} \sim W^{1/2})\ .$$

From (94) we see that on $[a,b] = [Z^{10^{-9}}, t_{\max}-20]$, we have $\tau(t) \geq 20$; $|t_1 - t_2| < c\tau(t_1)$ implies $\tau(t_1) \sim \tau(t_2)$ and $\sigma(t_1) \sim \sigma(t_2)$, since $t_1 \sim t_2$ and $t_{\max}-t_1 \sim t_{\max}-t_2$. Therefore, the hypotheses of the Lemma on Riemann sums are satisfied by $F(t)$, $\sigma(t)$, $\tau(t)$ on $[a,b]$. That Lemma yields

$$(95)\quad \sum_{Z^{10^{-9}} \leq \ell \leq t_{\max}-20} (2\ell+1)\big(W - \ell(\ell+1)\big)^{1/2} = \sum_{\ell \in [a,b]\cap\mathbb{Z}} F(\ell) = \int_a^b F(t)dt + \ \mathrm{Error}_1\ , \qquad \text{with}$$

$$(96)\qquad |\mathrm{Error}_1| \leq C\sigma(a) + C\sigma(b) + C\int_a^b \sigma(t)\tau^{-100}(t)dt\ .$$

From (94) we see that $\sigma(a) \sim W^{1/2} \cdot Z^{10^{-9}}$, $\sigma(b) \sim W^{3/4}$,

$$\int_a^{\frac{1}{2}t_{\max}} \sigma(t)\tau^{-100}(t)dt \sim \int_{Z^{10^{-9}}}^{\frac{1}{2}t_{\max}} [W^{1/2}t]\cdot t^{-100}dt \leq W^{1/2}\ ,$$

$$\int_{\frac{1}{2}t_{\max}}^{b} \sigma(t)\tau^{-100}(t)dt \sim \int_{\frac{1}{2}t_{\max}}^{t_{\max}-20} \left[W^{3/4}(t_{\max}-t)^{1/2}\right](t_{\max}-t)^{-100}dt$$
$$\sim W^{3/4} \ .$$

Putting these results into (96), we see that

$$|\text{Error}_1| \leq CW^{3/4} + CW^{1/2}Z^{10^{-9}} \ . \tag{97}$$

Also, $\int_a^b F(t)dt = \int_a^b (2t+1)\big(W - t(t+1)\big)^{1/2}dt = \int_{a(a+1)}^{b(b+1)} (W-u)^{1/2}du = \frac{2}{3}\big(W - a(a+1)\big)^{3/2} - \frac{2}{3}\big(W - b(b+1)\big)^{3/2}$. Here, $W - b(b+1) \sim W^{1/2}(t_{\max} - b) \sim W^{1/2}$, so $\big(W - b(b+1)\big)^{3/2} \leq CW^{3/4}$. Also $a(a+1) < (1.1)Z^{2\cdot 10^{-9}} < \frac{2}{3}W$, so $\left|\frac{2}{3}W^{3/2} - \frac{2}{3}\big(W - a(a+1)\big)^{3/2}\right| \leq CW^{1/2}a(a+1)$ (by the mean-value theorem) $\leq C'W^{1/2}Z^{2\cdot 10^{-9}}$. Therefore,

$$\int_a^b F(t)dt = \frac{2}{3}W^{3/2} + \ \text{Error}_2 \ , \text{with } |\text{Error}_2| \leq CW^{1/2}Z^{2\cdot 10^{-9}} + CW^{3/4} \ . \tag{98}$$

From (95), (97), (98), we get

$$\sum_{Z^{10^{-9}} \leq \ell \leq t_{\max}-20} (2\ell+1)\big(W - \ell(\ell+1)\big)^{1/2} = \frac{2}{3}W^{3/2} + \text{Error}_3 \ , \ \text{with} \tag{99}$$

$$|\text{Error}_3| \leq CW^{3/4} + CZ^{2\cdot 10^{-9}}W^{1/2} \ . \tag{100}$$

Since $t_{\max}$ is the positive root of $t(t+1) = W$, we have

$$\begin{aligned} \sum_{\ell \geq Z^{10^{-9}}} (2\ell+1)\big(W - \ell(\ell+1)\big)_+^{1/2} = &\left[\sum_{Z^{10^{-9}} \leq \ell \leq t_{\max}-20} (2\ell+1)\big(W - \ell(\ell+1)\big)^{1/2}\right] \\ &+ \left[\sum_{t_{\max}-20 < \ell < t_{\max}} (2\ell+1)\big(W - \ell(\ell+1)\big)^{1/2}\right] . \end{aligned} \tag{101}$$

The first sum on the right is controlled by (99). The second sum has at most 20 terms, each of which is dominated by $CW^{3/4}$ by virtue of (93), (94). Hence the second sum on the right of (101) is dominated by $CW^{3/4}$. So (99), (100), (101) imply $\sum_{\ell \geq Z^{10^{-9}}} (2\ell+1)\big(W-\ell(\ell+1)\big)_+^{1/2} = \frac{2}{3}W^{3/2} +$ Error, with $|\text{Error}| < CW^{3/4} + CZ^{2\cdot 10^{-9}}W^{1/2}$. This is the conclusion of Lemma 9, since $W > 2Z^{2\cdot 10^{-9}}$. ■

To control ρ_{sc} using Lemma 9, we simply recall the definitions (28), (33) to write

$$\begin{aligned}\rho_{sc}(r) &= \sum_{\ell \geq Z^{10^{-9}}} (2\ell+1)\cdot \frac{1}{\pi}\Big(-\frac{\ell(\ell+1)}{r^2} - V(r)\Big)_+^{1/2} \\ &= \frac{1}{\pi r} \sum_{\ell \geq Z^{10^{-9}}} (2\ell+1)\big(-r^2V(r) - \ell(\ell+1)\big)_+^{1/2} .\end{aligned}$$

Lemma 9, with $W = -r^2V(r)$, gives

$$\rho_{sc}(r) = \frac{2}{3\pi r}\big(-r^2V(r)\big)^{3/2}\chi_{{}_{-r^2V(r) > Z^{2\cdot 10^{-9}}}} + \tilde{\rho}_{\text{EXTRA}}(r) \text{ , with} \tag{102}$$

$$|\tilde{\rho}_{\text{EXTRA}}(r)| \leq C\chi_{{}_{-r^2V(r) > Z^{2\cdot 10^{-9}}}}\left\{\frac{\big(-r^2V(r)\big)^{3/4}}{r} + Z^{2\cdot 10^{-9}}\frac{\big(-r^2V(r)\big)^{1/2}}{r}\right\} . \tag{103}$$

We rewrite (102), (103) slightly as

$$\rho_{sc}(r) = 4\pi r^2 \cdot \frac{\big(-V(r)\big)^{3/2}}{6\pi^2}\chi_{{}_{-r^2V(r) > Z^{2\cdot 10^{-9}}}} + \tilde{\rho}_{\text{EXTRA}}(r) \ , \quad \text{or}$$

$$\rho_{sc}(r) = 4\pi r^2 \cdot \frac{\big(-V(r)\big)_+^{3/2}}{6\pi^2} + \rho_{\text{EXTRA}}(r) \ , \quad \text{with} \tag{104}$$

$$\begin{aligned}|\rho_{\text{EXTRA}}(r)| &\leq Cr^2\big(-V(r)\big)_+^{3/2}\chi_{{}_{-r^2V(r) \leq Z^{2\cdot 10^{-9}}}} \\ &+ C\frac{\big(-r^2V(r)\big)_+^{3/4}}{r}\cdot\chi_{{}_{-r^2V(r) > Z^{2\cdot 10^{-9}}}} + CZ^{2\cdot 10^{-9}}\frac{\big(-r^2V(r)\big)_+^{1/2}}{r}\chi_{{}_{-r^2V(r) > Z^{2\cdot 10^{-9}}}}\end{aligned} \tag{105}$$

These are our basic results on ρ_{sc}.

Next, we estimate ρ_{LOW}. Fix $\overline{C}$ as in Lemma 3. For $\overline{C} \leq \ell < Z^{10^{-9}}$, Lemma 3 and the Second Degenerate Density Lemma yield

(106)

$$\int_0^{Z^{-9/10}} \rho_\ell(r)dr \leq C + CZ^{-3/20}\int_0^\infty \big(-V_\ell(r)\big)_+^{1/2}dr + C\int_0^\infty \big(-Z^{18/10} - V_\ell(r)\big)_+^{1/2}dr$$

and

$$\int_0^\infty \rho_\ell(r)dr \le C + C\int_0^\infty \big(-V_\ell(r)\big)_+^{1/2} dr \ . \tag{107}$$

Since $V_\ell(r) = \frac{\ell(\ell+1)}{r^2} + V(r) > V(r) \sim -S(r)$ by (i), (ii), (2), (106) and (107) imply

$$\int_0^{Z^{-9/10}} \rho_\ell(r)dr \le C + CZ^{-3/20}\int_0^\infty S^{1/2}(r)dr + C\int_{S(r)>cZ^{18/10}} S^{1/2}(r)dr$$

and

$$\int_0^\infty \rho_\ell(r)dr \le C + C\int_0^\infty S^{1/2}(r)dr \ .$$

Recalling the definition of $S(r)$, we get

$$\int_0^{Z^{-9/10}} \rho_\ell(r)dr \le CZ^{11/60} \qquad \text{for} \quad \overline{C} \le \ell < Z^{10^{-9}} \tag{108}$$

$$\int_0^\infty \rho_\ell(r)dr \le CZ^{1/3} \qquad \text{for} \quad \overline{C} \le \ell < Z^{10^{-9}} \ . \tag{109}$$

Similarly, for $1 \le \ell < \overline{C}$ (with $\overline{C}$ as in Lemma 3), Lemma 2 and the Third Degenerate Density Lemma yield

$$\int_0^{Z^{-9/10}} \rho_\ell(r)dr \le C + CZ^{-3/20}\int_0^\infty \big(-V_\ell(r)\big)_+^{1/2} dr + C\int_0^\infty \big(E_{\text{crit}} - V_\ell(r)\big)_+^{1/2} dr \tag{110}$$

and

$$\int_0^\infty \rho_\ell(r)dr \le C + C\int_0^\infty \big(-V_\ell(r)\big)_+^{1/2} dr \ , \tag{111}$$

with $E_{\text{crit}} = V_\ell(Z^{-8/10})$. When $r = Z^{-8/10}$ and $\ell < \overline{C}$, we have $\frac{\ell(\ell+1)}{r^2} \le CZ^{16/10}$ and $V(r) \sim -S(r) = -Z^{18/10}$ by (i), (ii), (2). Thus $E_{\text{crit}} = V_\ell(Z^{-8/10}) \sim -Z^{18/10}$. Hence (110), (111) simply assert that (106), (107) hold for $1 \le \ell < \overline{C}$. Just as (106), (107) led to (108), (109), we now obtain

$$\int_0^{Z^{-9/10}} \rho_\ell(r)dr \le CZ^{11/60} \quad \text{for} \quad 1 \le \ell < \overline{C} \tag{112}$$

$$(113)\qquad \int_0^\infty \rho_\ell(r)dr \le CZ^{1/3} \qquad \text{for} \quad 1 \le \ell < \overline{C}\ .$$

For $\ell = 0$, Lemma 1 and the Fourth Degenerate Density Lemma yield

$$\int_0^{Z^{-9/10}} \rho_\ell(r)dr \le C + CZ^{-3/20}\int_0^\infty \big(-V(r)\big)_+^{1/2}dr + C\int_0^\infty \big(E_{\text{crit}} - V(r)\big)_+^{1/2}dr$$

and

$$\int_0^\infty \rho_\ell(r)dr \le C + C\int_0^\infty \big(-V(r)\big)_+^{1/2}dr\ ,$$

with $E_{\text{crit}} = V(Z^{-8/10}) \sim -S(Z^{-8/10}) = -Z^{18/10}$. So once again we obtain

$$(114)\qquad \int_0^{Z^{-9/10}} \rho_\ell(r)dr \le CZ^{11/60} \quad \text{for} \quad \ell = 0$$

$$(115)\qquad \int_0^\infty \rho_\ell(r)dr \le CZ^{1/3} \quad \text{for} \quad \ell = 0\ .$$

Putting (108), (109), (112), (113), and (114), (115) into the definition of $\rho_{\text{LOW}}(r)$, we obtain the estimates:

$$\int_0^{Z^{-9/10}} \rho_{\text{LOW}}(r)dr \le CZ^{\frac{11}{60}} \cdot Z^{2\cdot 10^{-9}}$$

$$\int_0^\infty \rho_{\text{LOW}}(r)dr \le CZ^{1/3} \cdot Z^{2\cdot 10^{-9}}\ .$$

Thus,

$$(116)\qquad \int_0^R \rho_{\text{LOW}}(r)dr \le CZ^{\frac{11}{60}+2\cdot 10^{-9}} + C\chi_{R>Z^{-9/10}} Z^{\frac{1}{3}+2\cdot 10^{-9}}\ .$$

This is our basic estimate for ρ_{LOW}.

At last we have learned enough to draw conclusions about the three-dimensional density ρ. From (31) and (104) we have

$$(117)\quad 4\pi r^2\Big[\rho(r) - \frac{1}{6\pi^2}\big(-V(r)\big)_+^{3/2}\Big] = \rho_{\text{LOW}}(r) + \rho_{\text{EXTRA}}(r) + \rho_{NT}(r) + \rho_{\text{ERROR}}(r)\ .$$

The integrals of $\rho_{\mathrm{LOW}}(r)$, $\rho_{\mathrm{EXTRA}}(r)$, $\rho_{NT}(r)$, on $[0,R]$ are estimated by (116), (105) and (86). Hence we obtain

(118)

$$\Big|\int_0^R [\rho_{\mathrm{LOW}}(r)+\rho_{\mathrm{EXTRA}}(r)+\rho_{NT}(r)]dr\Big| \le \big[CZ^{\frac{11}{60}+2\cdot 10^{-9}} + C\chi_{_{R>Z^{-9/10}}} Z^{\frac{1}{3}+2\cdot 10^{-9}}\big]$$
$$+\big[C\int_0^R r^2\big(-V(r)\big)_+^{3/2}\chi_{_{-r^2V(r)\le Z^{2\cdot 10^{-8}}}}dr + C\int_0^R \big(-r^2V(r)\big)_+^{3/4}\chi_{_{-r^2V(r)>Z^{2\cdot 10^{-9}}}}\frac{dr}{r}$$
$$+CZ^{2\cdot 10^{-9}}\int_0^R\big(-r^2V(r)\big)_+^{1/2}\chi_{_{-r^2V(r)>Z^{2\cdot 10^{-9}}}}\frac{dr}{r}\big]$$
$$+\big[C\chi_{_{R>c\check{r}}}\Omega^{2-2a}+C\int_0^{2R}\big(-r^2V(r)\big)_+^{1-a}\frac{dr}{r}+C\int_0^{2R}\min\{\big(-r^2V(r)\big)_+, c\Omega^{2-8a}\}\frac{dr}{r}\big]\ .$$

(For convenience, we have harmlessly changed a 10^{-9} to 10^{-8} in (118). This merely weakens the estimate.)

We will check that several of the terms on the right-hand side of (118) may be dropped, because they are dominated by the remaining terms on the right.

In fact,

(119)
$$Z^{2\cdot 10^{-9}}\int_0^R\big(-r^2V(r)\big)_+^{1/2}\chi_{_{-r^2V(r)>Z^{2\cdot 10^{-9}}}}\frac{dr}{r}$$
$$\le \int_0^R r^2\big(-V(r)\big)_+^{3/2}\chi_{_{-r^2V(r)\le Z^{2\cdot 10^{-8}}}}dr+\int_0^R\big(-r^2V(r)\big)_+^{3/4}\chi_{_{-r^2V(r)>Z^{2\cdot 10^{-9}}}}\frac{dr}{r}$$

(120)
$$\int_0^R\big(-r^2V(r)\big)_+^{3/4}\chi_{_{-r^2V(r)>Z^{2\cdot 10^{-9}}}}\frac{dr}{r}\le\int_0^{2R}\big(-r^2V(r)\big)_+^{1-a}\frac{dr}{r}$$

(121)
$$\int_0^R r^2\big(-V(r)\big)_+^{3/2}\chi_{_{-r^2V(r)\le Z^{2\cdot 10^{-8}}}}dr$$
$$\le C\int_0^R r^2S^{3/2}(r)\chi_{_{r^2S(r)\le CZ^{2\cdot 10^{-8}}}}dr\le CZ^{3\cdot 10^{-8}}\ \text{(by (0))}$$
$$\le CZ^{\frac{11}{60}+2\cdot 10^{-9}}\ .$$

Hence on the right-hand side of (118) we may delete the left-hand side of (119), (120), (121) without changing the total order of magnitude. Thus, (118) becomes

$$\Big|\int_0^R [\rho_{\mathrm{LOW}}(r)+\rho_{\mathrm{EXTRA}}(r)+\rho_{NT}(r)]dr\Big|$$
$$\le CZ^{\frac15}+C\chi_{R>Z^{-9/10}}\cdot Z^{\frac13+2\cdot10^{-9}}+CZ^{\frac23-\frac23 a}\,\chi_{R>cZ^{-\frac13}}$$
$$+C\int_0^{2R}\big(-r^2V(r)\big)_+^{1-a}\frac{dr}{r}+C\int_0^{2R}\min\{\big(-r^2V(r)\big)_+,cZ^{\frac23-\frac83 a}\}\frac{dr}{r}\ .$$

(Here we dominated $Z^{\frac{11}{60}+2\cdot10^{-9}}$ by $Z^{\frac{12}{60}}=Z^{1/5}$, and we recalled that $\Omega\sim Z^{1/3}$, $\check r\sim Z^{-1/3}$.)

This implies trivially that

$$(122)\quad \Big(Av_{|R-R_0|<\frac{1}{10}R_0}\Big|\int_0^R [\rho_{\mathrm{LOW}}(r)+\rho_{\mathrm{EXTRA}}(r)+\rho_{NT}(r)]dr\Big|^2\Big)^{1/2}$$
$$\le CZ^{\frac15}+C\chi_{R_0>\frac12 Z^{-9/10}}\cdot Z^{\frac13+2\cdot10^{-9}}+CZ^{\frac23-\frac23 a}\chi_{R_0>cZ^{-1/3}}$$
$$+C\int_0^{4R_0}\big(-r^2V(r)\big)_+^{1-a}\frac{dr}{r}+C\int_0^{4R_0}\min\{\big(-r^2V(r)\big)_+,cZ^{\frac23-\frac83 a}\}\frac{dr}{r}\ .$$

This estimate can be combined with estimate (46) for ρ_{ERROR}. In view of (117), we obtain the following result.

$$\Big(Av_{|R-R_0|<\frac{1}{10}R_0}\Big|\int_0^R [\rho(r)-\frac{1}{6\pi^2}(-V(r))_+^{3/2}]4\pi r^2dr\Big|^2\Big)^{1/2}$$
$$\le \Big[CZ^{\frac15}+CZ^{\frac13+2\cdot10^{-9}}\chi_{R_0>\frac12 Z^{-9/10}}+CZ^{\frac23-\frac23 a}\chi_{R_0>cZ^{-1/3}}$$
$$+C\int_0^{4R_0}\big(-r^2V(r)\big)_+^{1-a}\frac{dr}{r}+C\int_0^{4R_0}\min\{(-r^2V(r))_+,cZ^{\frac23-\frac83 a}\}\Big]$$
$$+\Big[Z^{10-N}+CZ^{\frac23-\frac23 a}\chi_{R_0>cZ^{-1/3}}$$
$$+C\int_0^{2R_0}\big(-r^2V(r)\big)_+^{1-a}\frac{dr}{r}+C\int_0^{2R_0}\big(-r^2V(r)\big)_+\chi_{-r^2V(r)<CZ^{\frac23-\frac83 a}}\frac{dr}{r}\Big]\ .$$

Each of the last four terms on the right is dominated by one of the previous terms on the right. Hence, the above estimate may be rewritten as

$$(123)\quad \Big(Av_{|R-R_0|<\frac{1}{10}R_0}\Big|\int_0^R [\rho(r)-\frac{1}{6\pi^2}\big(-V(r)\big)_+^{3/2}]4\pi r^2dr\Big|^2\Big)^{1/2}$$
$$\le CZ^{\frac15}+CZ^{\frac13+2\cdot10^{-9}}\chi_{R_0>\frac12 Z^{-9/10}}+CZ^{\frac23-\frac23 a}\chi_{R_0>cZ^{-1/3}}$$
$$+C\int_0^{4R_0}\big(-r^2V(r)\big)_+^{1-a}\frac{dr}{r}+C\int_0^{4R_0}\min\{\big(-r^2V(r)\big)_+,cZ^{\frac23-\frac83 a}\}\frac{dr}{r}\ .$$

The right-hand side simplifies further. For $r \sim Z^{-1/3}$ we have $-r^2V(r) \sim r^2S(r) = Zr \sim Z^{2/3}$, so that $Z^{\frac{2}{3}-\frac{2}{3}a}\chi_{_{R_0>cZ^{-1/3}}} \le C\int_0^{4R_0}\big(-r^2V(r)\big)_+^{1-a}\frac{dr}{r}$. Thus, the term $CZ^{\frac{2}{3}-\frac{2}{3}a}\chi_{_{R_0>cZ^{-1/3}}}$ may be deleted from (123).

Also,

$$\begin{aligned}
\int_0^{4R_0}\big(-r^2V(r)\big)_+^{1-a}\frac{dr}{r} &\le \int_0^{\infty}\big(-r^2V(r)\big)_+^{1-a}\chi_{_{-r^2V(r)<1}}\frac{dr}{r} \\
&\quad + \int_0^{4R_0}\chi_{_{-r^2V(r)\ge 1}}\cdot\min\{\big(-r^2V(r)\big)_+, C\Omega^{2(1-a)}\}\frac{dr}{r} \\
&\le C\int_0^{\infty}\big(r^2S(r)\big)^{1-a}\chi_{_{r^2S(r)<C}}\frac{dr}{r} + C\int_0^{4R_0}\min\{\big(-r^2V(r)\big)_+, \Omega^{2-2a}\}\frac{dr}{r} \\
&= \Big[C\int_0^{Z^{-1/3}}(Zr)^{1-a}\chi_{_{Zr<C}}\frac{dr}{r} + C\int_{Z^{-1/3}}^{\infty}(r^{-2})^{1-a}\chi_{_{r^{-2}<C}}\frac{dr}{r}\Big] \\
&\quad + C\int_0^{4R_0}\min\{\big(-r^2V(r)\big), Z^{\frac{2}{3}-\frac{2}{3}a}\}\frac{dr}{r}\ , \\
&\le C' + C\int_0^{4R_0}\min\{\big(-r^2V(r)\big), Z^{\frac{2}{3}-\frac{2}{3}a}\}\frac{dr}{r}\ .
\end{aligned}$$

So the terms $\int_0^{4R_0}\big(-r^2V(r)\big)_+^{1-a}\frac{dr}{r}$ and $\int_0^{4R_0}\min\{\big(-r^2V(r)\big), Z^{\frac{2}{3}-\frac{8}{3}a}\}\frac{dr}{r}$ are both dominated by $\int_0^{4R_0}\min\{\big(-r^2V(r)\big), Z^{\frac{2}{3}-\frac{2}{3}a}\}\frac{dr}{r} + CZ^{1/5}$. Consequently, (123) may be rewritten in the form

$$\begin{aligned}
&(124)\quad \Big(Av_{|R-R_0|<\frac{1}{10}R_0}\Big|\int_0^R[\rho(r) - \frac{1}{6\pi^2}\big(-V(r)\big)^{3/2}]4\pi r^2dr\Big|^2\Big)^{1/2} \\
&\qquad \le CZ^{1/5} + CZ^{\frac{1}{3}+2\cdot 10^{-9}}\chi_{_{R_0>\frac{1}{2}Z^{-9/10}}} + C\int_0^{4R_0}\min\{r^2S(r), Z^{\frac{2}{3}-\frac{2}{3}a}\}\frac{dr}{r}\ .
\end{aligned}$$

By definition (0),

$$\min\{r^2S(r), Z^{\frac{2}{3}-\frac{2}{3}a}\} = \begin{cases} Zr & \text{if } 0 < r \le Z^{-\frac{1}{3}-\frac{2}{3}a} \\ Z^{\frac{2}{3}-\frac{2}{3}a} & \text{if } Z^{-\frac{1}{3}-\frac{2}{3}a} \le r \le Z^{-\frac{1}{3}+\frac{a}{3}} \\ r^{-2} & \text{if } Z^{-\frac{1}{3}+\frac{a}{3}} \le r < \infty \end{cases}$$

so

$$\int_0^{4R_0}\min\{r^2S(r), Z^{\frac{2}{3}-\frac{2}{3}a}\}\frac{dr}{r} \sim \begin{cases} ZR_0 & \text{if } 0 < R_0 \le Z^{-\frac{1}{3}-\frac{2}{3}a} \\ Z^{\frac{2}{3}-\frac{2}{3}a}\ \ell n\big(\frac{CR_0}{Z^{-\frac{1}{3}-\frac{2}{3}a}}\big) & \text{if } Z^{-\frac{1}{3}-\frac{2}{3}a} \le R_0 \le Z^{-1/3+a/3} \\ Z^{\frac{2}{3}-\frac{2}{3}a}[1 + a\,\ell n\ Z] & \text{if } Z^{-1/3+a/3} \le R_0 < \infty \end{cases}.$$

Hence (124) becomes

$$(125)\qquad \Big(Av_{|R-R_0|<\frac{1}{10}R_0}\Big|\int_0^R[\rho(r)-\frac{1}{6\pi^2}\big(-V(r)\big)^{3/2}]4\pi r^2dr\Big|^2\Big)^{1/2}\le C\mathcal{E}_a(R_0)$$

with

$$(126)\qquad \mathcal{E}_a(R_0)=Z^{\frac{1}{5}}\quad\text{for}\quad 0<R_0<\frac{1}{2}Z^{-\frac{9}{10}}$$

$$(127)\qquad \mathcal{E}_a(R_0)=Z^{\frac{1}{3}+2\cdot 10^{-9}}\quad\text{for}\quad \frac{1}{2}\,Z^{-\frac{9}{10}}\le R_0\le Z^{-\frac{2}{3}+2\cdot 10^{-9}}$$

$$(128)\qquad \mathcal{E}_a(R_0)=ZR_0\quad\text{for}\quad Z^{-\frac{2}{3}+2\cdot 10^{-9}}\le R_0\le Z^{-\frac{1}{3}-\frac{2}{3}a}$$

$$(129)\qquad \mathcal{E}_a(R_0)=Z^{\frac{2}{3}-\frac{2}{3}a}(1+\ell n[Z^{\frac{1}{3}+\frac{2}{3}a}R_0])\quad\text{for } Z^{-\frac{1}{3}-\frac{2}{3}a}\le R_0\le Z^{-\frac{1}{3}+\frac{1}{3}a}$$

$$(130)\qquad \mathcal{E}_a(R_0)=Z^{\frac{2}{3}-\frac{2}{3}a}(1+a\,\ell nZ)\quad\text{for } Z^{-\frac{1}{3}+\frac{1}{3}a}\le R_0<\infty\ .$$

Estimates (125)...(130) are our basic results for the three-dimensional density ρ associated to $-\Delta+V$.

The next two lemmas are elementary consequences of (125)...(130).

Lemma 10. *Suppose $U(r)$ is a smooth function supported in $\{\delta r<r<2\delta\}$ and satisfying $|U(r)|\le C$, $|U'(r)|\le C\delta^{-1}$. Assume $\delta<Z^{-1/3}$. Then*

$$\Big|\int_0^\infty U(r)\rho(r)4\pi r^2dr-\int_0^\infty U(r)\cdot\frac{\big(-V(r)\big)^{3/2}}{6\pi^2}4\pi r^2dr\Big|\le C\mathcal{E}_0(C\delta)\ .$$

Proof. We use (125)...(130) with $a=0$. In particular, we don't need to assume number-theoretic type a for $a>0$. (See (24)...(26)). With

$$G(R)=\int_0^R[\rho(r)-\frac{\big(-V(r)\big)^{3/2}}{6\pi^2}]4\pi r^2dr\ ,$$

we have

$$
\begin{aligned}
&\Big|\int_0^\infty U(r)\rho(r)4\pi r^2 dr - \int_0^\infty U(r)\cdot\frac{\big(-V(r)\big)^{3/2}}{6\pi^2}4\pi r^2 dr\Big| \\
&\qquad = \Big|\int_0^\infty U(r)G'(r)dr\Big| = \Big|\int_0^\infty U'(r)G(r)dr\Big| \\
&\qquad \le C\int_0^\infty \Big(\frac{1}{R_0}\int_{|R-R_0|<\frac{1}{10}R_0} |U'(R)|\ |G(R)|dR\Big)dR_0 \\
&\le C\int_0^\infty \Big(\frac{1}{R_0}\int_{|R-R_0|<\frac{1}{10}R_0} |U'(R)|^2 dR\Big)^{1/2}\Big(\frac{1}{R_0}\int_{|R-R_0|<\frac{1}{10}R_0} |G(R)|^2 dR\Big)^{1/2} dR_0 \\
&\qquad \le C\int_0^\infty \delta^{-1}\chi_{c\delta<R_0<C\delta}\mathcal{E}_0(R_0)dR_0
\end{aligned}
$$

(by (125), and by our assumptions on $U(R)$) $\le C\mathcal{E}_0(C\delta)$. ■

Lemma 11. *We have the estimate*

$$
\int_0^\infty \Big|\int_0^R [\rho(r) - \frac{\big(-V(r)\big)^{3/2}}{6\pi^2}]4\pi r^2 dr\Big|^2 \frac{dR}{Z^{-2}+R^2} \le CZ^{\frac{5}{3}-\frac{2}{3}a} .
$$

Proof. With $G(R) = \int_0^R [\rho(r) - \frac{\left(-V(r)\right)^{3/2}}{6\pi^2}]4\pi r^2 dr$, we have

$$
\begin{aligned}
\int_0^\infty |G(R)|^2 \frac{dR}{Z^{-2}+R^2} &\le C\int_0^\infty \Big(\frac{1}{R_0}\int_{|R-R_0|<\frac{1}{10}R_0} \frac{|G(R)|^2}{Z^{-2}+R^2}dR\Big)dR_0 \\
&\le C\int_0^\infty \Big(\frac{1}{R_0}\int_{|R-R_0|<\frac{1}{10}R_0} |G(R)|^2 dR\Big)\frac{dR_0}{Z^{-2}+R_0^2} \\
&\le C\int_0^\infty (\mathcal{E}_a(R_0))^2 \frac{dR_0}{Z^{-2}+R_0^2} \quad \text{by (125)} .
\end{aligned}
$$

Now (126)...(130) yield:

$$
\int_0^{\frac{1}{2}Z^{-9/10}} (\mathcal{E}_a(R_0))^2 \frac{dR_0}{Z^{-2}+R_0^2} \le Z^{\frac{2}{5}}\int_0^\infty \frac{dR_0}{Z^{-2}+R_0^2} = CZ^{\frac{7}{5}} << Z^{\frac{5}{3}-\frac{2}{3}a} ;
$$

$$
\int_{\frac{1}{2}Z^{-9/10}}^{Z^{-\frac{2}{3}+2\cdot 10^{-9}}} (\mathcal{E}_a(R_0))^2 \frac{dR_0}{Z^{-2}+R_0^2} \le Z^{\frac{2}{3}+4\cdot 10^{-9}}\int_{\frac{1}{2}Z^{-\frac{9}{10}}}^\infty \frac{dR_0}{R_0^2} = CZ^{\frac{5}{3}-\frac{1}{10}+4\cdot 10^{-9}} << Z^{\frac{5}{3}-\frac{2}{3}a} ;
$$

$$
\int_{Z^{-\frac{2}{3}+2\cdot 10^{-9}}}^{Z^{-\frac{1}{3}-\frac{2}{3}a}} (\mathcal{E}_a(R_0))^2 \frac{dR_0}{Z^{-2}+R_0^2} \le \int_0^{Z^{-\frac{1}{3}-\frac{2}{3}a}} (ZR_0)^2 \frac{dR_0}{R_0^2} = Z^{\frac{5}{3}-\frac{2}{3}a} ;
$$

$$\int_{Z^{-\frac{1}{3}-\frac{2}{3}a}}^{Z^{-\frac{1}{3}+\frac{1}{3}a}} (\mathcal{E}_a(R_0))^2 \frac{dR_0}{Z^{-2}+R_0^2}$$
$$\leq \int_{Z^{-\frac{1}{3}-\frac{2}{3}a}}^{\infty} Z^{\frac{4}{3}-\frac{4}{3}a}(1+\ell n[Z^{\frac{1}{3}+\frac{2}{3}a}R_0])^2 \frac{dR_0}{R_0^2}$$
$$= Z^{\frac{4}{3}-\frac{4}{3}a} \cdot Z^{\frac{1}{3}+\frac{2}{3}a} \int_1^{\infty} (1+\ell n\, t)^2 \frac{dt}{t^2} \leq C Z^{\frac{5}{3}-\frac{2}{3}a} \ ;$$

$$\int_{Z^{-\frac{1}{3}+\frac{1}{3}a}}^{\infty} (\mathcal{E}_a(R_0))^2 \frac{dR_0}{Z^{-2}+R_0^2} \leq \int_{Z^{-\frac{1}{3}+\frac{1}{3}a}}^{\infty} Z^{\frac{4}{3}-\frac{4}{3}a}(1+a\,\ell n Z)^2 \frac{dR_0}{R_0^2}$$
$$= Z^{\frac{4}{3}-\frac{4}{3}a}(1+a\,\ell n\, Z)^2 \cdot Z^{+\frac{1}{3}-\frac{1}{3}a} = Z^{\frac{5}{3}-\frac{5}{3}a}(1+a\,\ell n\, Z)^2 \leq C Z^{\frac{5}{3}-\frac{2}{3}a} \ .$$

Hence, $\int_0^\infty |G(R)|^2 \frac{dR}{Z^{-2}+R^2} \leq C \int_0^\infty (\mathcal{E}_a(R_0))^2 \frac{dR_0}{Z^{-2}+R_0^2} \leq C Z^{\frac{5}{3}-\frac{2}{3}a}$, which is the conclusion of the Lemma. ■

In Lemma 11, we want to replace $(Z^{-2}+R^2)$ by R^2. If we simply use (125)...(130) and try to repeat the proof of Lemma 11, then we get a divergent integral because of the singularity at $R=0$. This reflects our lack of attention to the vanishing of $\int_0^R [\rho(r) - \frac{1}{6\pi^2}\big(-V(r)\big)^{3/2}] 4\pi r^2 dr$ at $R=0$. To remedy the problem at the origin, it is convenient to return to $\mathbb{R}^3$, and invoke the following elementary elliptic estimate.

Lemma 12. *Suppose $-\Delta u = Wu$ on $\mathbb{R}^3$, with $|W(x)| \leq \frac{C}{|x|}$ on the ball $B(0,3)$. Then*

$$\|u\|_{L^\infty(B(0,1))} \leq C\|u\|_{L^2(B(0,3))} \ .$$

Proof. The Sobolev and Hölder inequalities give

$$\text{(131)} \qquad \|u\|_{L^\infty(B(0,1))} \leq C\|\Delta u\|_{L^{30/17}(B(0,2))} + C\|u\|_{L^5(B(0,2))}$$

$$\text{(132)} \qquad \|\Delta u\|_{L^{30/17}(B(0,2))} = \|Wu\|_{L^{30/17}(B(0,2))} \leq \|W\|_{L^{\frac{30}{11}}(B(0,2))} \|u\|_{L^5(B(0,2))}$$

$$\text{(133)} \qquad \|u\|_{L^5(B(0,2))} \leq C\|\Delta u\|_{L^{15/13}(B(0,3))} + C\|u\|_{L^2(B(0,3))}$$

(134) $$\|\Delta u\|_{L^{15/13}(B(0,3))} = \|Wu\|_{L^{15/13}(B(0,3))} \leq \|W\|_{L^{\frac{30}{11}}(B(0,3))} \|u\|_{L^2(B(0,3))} \ .$$

Since $\|W\|_{L^{30/11}(B(0,3))} \leq C$, estimates (131) and (132) show that

(135) $$\|u\|_{L^\infty(B(0,1))} \leq C\|u\|_{L^5(B(0,2))} \ ;$$

and estimates (133) and (134) show that

(136) $$\|u\|_{L^5(B(0,2))} \leq C\|u\|_{L^2(B(0,3))} \ .$$

The conclusion of the Lemma is immediate from (135), (136). ■

The indices here are somewhat arbitrary, and the proof is very old. Rescaling from the unit ball to $B(0, Z^{-1})$ by setting $\tilde{u}(x) = u(Z^{-1}x)$ for $u \in L^2(B(0, Z^{-1}))$, we get from Lemma 12 the following result.

Corollary 1. *Suppose $\Delta u = Wu$ and $|W(x)| \leq \frac{CZ}{|x|}$ on $B(0, 3Z^{-1}) \subset \mathbb{R}^3$. Then*

$$\max_{x \in B(0,Z^{-1})} |u(x)|^2 \leq CZ^3 \int_{B(0,3Z^{-1})} |u(x)|^2 dx \ .$$

This in turn implies

Corollary 2. *Let E_k be the non-positive eigenvalues of $-\Delta + W(x)$ on $\mathbb{R}^3$, and let $\psi_k(x)$ be the corresponding normalized eigenfunctions. Form the density $\rho(x) = \sum_k |\psi_k(x)|^2$ on $\mathbb{R}^3$. If $|W(x)| \leq \frac{CZ}{|x|}$ on $\mathbb{R}^3$ then $\max_{x \in B(0,Z^{-1})} \rho(x) \leq CZ^3 \int_{B(0,3Z^{-1})} \rho(x) dx$.* ■

Proof. The E_k are all bounded in absolute value by CZ^2, since $-\Delta + W \geq -\Delta - \frac{CZ}{|x|}$. Hence $|W(x) - E_k| \leq \frac{CZ}{|x|}$ on $B(0, 3Z^{-1})$. Apply the preceding corollary to each $\psi_k(x)$, and sum on k. ■

Let us return to functions of one variable. Corollary 2 says that

(137) $$\max_{0<r<Z^{-1}} \rho(r) \leq CZ^3 \int_0^{3Z^{-1}} \rho(r) 4\pi r^2 dr \ .$$

We can estimate the right-hand side by using (125), (126). In fact, from (125), (126) with $R_0 = 20Z^{-1}$, we get

$$\Big|\int_0^R [\rho(r) - \frac{\big(-V(r)\big)_+^{3/2}}{6\pi^2}] 4\pi r^2 dr\Big| \le CZ^{1/5}$$

$$\text{for at least one } R \text{ with } |R - R_0| < \frac{1}{10}R_0 \ , \ \text{hence } 10Z^{-1} < R < 30Z^{-1} \ .$$

Since also

$$\int_0^{30Z^{-1}} \big(-V(r)\big)^{3/2} r^2 dr \le C \int_0^{30Z^{-1}} S^{3/2}(r) r^2 dr = C \int_0^{30Z^{-1}} Z^{3/2} r^{1/2} dr \le C' \ ,$$

this implies

$$\int_0^R \rho(r) 4\pi r^2 dr \le CZ^{1/5} \ ,$$

hence

$$\int_0^{10Z^{-1}} \rho(r) 4\pi r^2 dr \le CZ^{1/5} \ .$$

Putting this into (137), we find that

$$\rho(r) \le CZ^{16/5} \quad \text{for} \quad 0 < r < Z^{-1} \ . \tag{138}$$

Hence

$$\int_0^{Z^{-1}} \Big|\int_0^R \rho(r)\cdot 4\pi r^2 dr\Big|^2 \frac{dR}{R^2} \le C \int_0^{Z^{-1}} (Z^{\frac{16}{5}} R^3)^2 \frac{dR}{R^2} = CZ^{\frac{32}{5}} \int_0^{Z^{-1}} R^4 dR = C' Z^{\frac{7}{5}} \ . \tag{139}$$

Since also

$$\int_0^{Z^{-1}} \Big|\int_0^R \frac{\big(-V(r)\big)^{3/2}}{6\pi^2} \cdot 4\pi r^2 dr\Big|^2 \frac{dR}{R^2} \le C \int_0^{Z^{-1}} \Big(\int_0^R Z^{3/2} r^{1/2} dr\Big)^2 \frac{dR}{R^2} = C \int_0^{Z^{-1}} (Z^3 R^3) \frac{dR}{R^2} = CZ^3 \int_0^{Z^{-1}} R dR = CZ \ ,$$

it follows from (139) that

$$\int_0^{Z^{-1}} \Big| \int_0^R [\rho(r) - \frac{\big(-V(r)\big)^{3/2}}{6\pi^2}] 4\pi r^2 dr \Big|^2 \frac{dR}{R^2} \leq C Z^{7/5}.$$

This inequality and Lemma 11 show that

$$\int_0^{\infty} \Big| \int_0^R [\rho(r) - \frac{\big(-V(r)\big)^{3/2}}{6\pi^2}] 4\pi r^2 dr \Big|^2 \frac{dR}{R^2} \leq C Z^{\frac{5}{3}-\frac{2}{3}a} \ . \tag{140}$$

Equation (140) has a three-dimensional interpretation. In fact, let E be the potential energy

$$\frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{f(x) f(y)}{|x-y|} \ dxdy$$

associated to a radially symmetric charge density f on $\mathbb{R}^3$. Then E is expressed in terms of the corresponding function $f(r)$ on $(0, \infty)$ by the formula

$$E = \frac{1}{2} \int_0^{\infty} \Big| \int_0^R f(r) \cdot 4\pi r^2 dr \Big|^2 \frac{dR}{R^2} \ .$$

This follows immediately by integrating Newton's formula

$$\int_{x \in S(R_1)} \int_{y \in S(R_2)} \frac{d\,\text{area}(x) \ d\,\text{area}(y)}{|x-y|} = \frac{(4\pi R_1^2)(4\pi R_2^2)}{\max(R_1, R_2)} \ ,$$

$$S(R) = \text{ sphere of radius } R \ .$$

Hence, (140) means that

$$\rho_{\text{err}}(x) = \rho(x) - \frac{1}{6\pi^2} \big(-V(x)\big)^{3/2} \quad \text{on } \mathbb{R}^3 \tag{141}$$

satisfies

$$\int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_{\text{err}}(x) \rho_{\text{err}}(y)}{|x-y|} \ dxdy \leq C Z^{\frac{5}{3}-\frac{2}{3}a} \ . \tag{142}$$

For future reference, we record (141), (142) and Lemma 10 above, in the next section.

The WKB Density Theorems for Approximate TF Potentials

Let $V_Z^{\mathrm{TF}}(x)$ be the Thomas-Fermi potential on $\mathbb{R}^3$. Thus $-\Delta V_Z^{\mathrm{TF}} = (\mathrm{const.})|V_Z^{\mathrm{TF}}|^{3/2}$ on $\mathbb{R}^3 \backslash \{0\}$, and

$$V_Z^{TF}(x) = -\frac{Z}{|x|} + O(1) \quad \text{as } x \to 0 \ .$$

Let $V(x)$ be a radially symmetric potential on $\mathbb{R}^3$. We write also $V(r)$, $V_Z^{\mathrm{TF}}(r)$ as functions of one variable. Assume

$$\text{(1)} \qquad \Big|\big(\frac{d}{dr}\big)^{\alpha} V(r)\Big| \leq C_\alpha r^{-\alpha} \min\{\frac{Z}{r}, r^{-4}\} \quad \text{for } \alpha \geq 0 \ ,$$

$$\text{(2)} \qquad \Big|\big(\frac{d}{dr}\big)^{\alpha} \{V(r) - V_Z^{\mathrm{TF}}(r)\}\Big| \leq c_0 r^{-\alpha} \min\{\frac{Z}{r}, r^{-4}\} \quad \text{for } 0 \leq \alpha \leq 2 \ ,$$

with c_0 a small positive constant determined by the C_α in (1).

Form the Schrödinger operator $H = -\Delta + V(x)$ on $\mathbb{R}^3$. Let E_k be the non-positive eigenvalues of H, and let $\psi_k(x)$ be the corresponding (normalized) eigenfunctions. As usual, form the density

$$\rho(x) = \sum_k |\psi_k(x)|^2 \quad \text{on } \mathbb{R}^3 \ .$$

Then define $\rho_{\mathrm{error}}(x) = \rho(x) - \frac{1}{6\pi^2}\big(-V(x)\big)_+^{3/2}$. Our goal is to estimate $\rho_{\mathrm{error}}(x)$.

Theorem 1. *Let $U(x)$ be a smooth, radially symmetric function on $\mathbb{R}^3$, supported in $\{\delta < |x| < 2\delta\}$ with $\delta < Z^{-1/3}$, and satisfying $|U(x)| \leq C$, $|\nabla U(x)| \leq C\delta^{-1}$. Assume Z is greater than a certain large, positive constant determined by the C_α in (1).*

Then

$$\Big|\int_{\mathbb{R}^3} U(x)\rho_{\mathrm{error}}(x)dx\Big| \leq C' Z\delta + C' Z^{\frac{1}{3}+2\cdot 10^{-9}} \ .$$

The constant C' depends only on C above, and on the C_α in (1).

Proof. This is a weakened form of Lemma 10 in the previous section. ∎

For a more refined estimate, we introduce Ω, the positive root $\Omega(\Omega+1) = \max_{r>0}\big(-r^2 V(r)\big)$. Thus $\Omega \sim Z^{1/3}$. For integers $0 \le \ell < \Omega$, we define

$$n_\ell = \int_0^\infty \Big(-V(r) - \frac{\ell(\ell+1)}{r^2}\Big)_+^{-1/2}\, dr \quad \text{and}$$

$$\phi_\ell = \frac{1}{\pi}\int_0^\infty \Big(-V(r) - \frac{\ell(\ell+1)}{r^2}\Big)_+^{1/2} dr - \frac{1}{2}\,.$$

Theorem 2. *Suppose the numbers, n_ℓ, ϕ_ℓ satisfy the following conditions, with $0 \le a < 1/43$.*

(A) *There are at most $C\Omega^{1-6a}$ integers $\ell \le \Omega$ for which $|\phi_\ell -$ (nearest integer)$| \le \ell^{-6/43}$.*

(B) *For $Z^{10^{-9}} \le \ell_1 < \ell_2 < \Omega$ with $\ell_2 - \ell_1 > \Omega^{1-10a}$, we have*

$$\Big| \sum_{\ell_1 \le \ell \le \ell_2} \frac{(2\ell+1)}{n_\ell} \chi_-(\phi_\ell) \Big| \le C\Omega^{-2a} \sum_{\ell_1 \le \ell \le \ell_2} \frac{(2\ell+1)}{n_\ell}\,.$$

Finally, suppose Z is greater than a certain large, positive constant determined by C, a in (A), (B); and by the C_α in (1).

Then $\int_{\mathbb{R}^3\times\mathbb{R}^3} \rho_{\mathrm{error}}(x)\rho_{\mathrm{error}}(y)\frac{dx\,dy}{|x-y|} \le C' Z^{\frac{5}{3}-\frac{2}{3}a}$. The constant C' depends only on C, a and the C_α in (1).

Proof. (A) and (B) imply (24)…(26) in the previous section, so our Lemma is just (142) of that section. ■

Clearly, we shall have to do some work to establish (A) and (B) for a positive a. Note that the analogues of (A) and (B) are false for the harmonic oscillator and for the Hydrogen atom, as mentioned in the introduction.

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