THE EIGENVALUE SUM FOR A THREE-DIMENSIONAL RADIAL POTENTIAL

by

C. Fefferman* **and** **L. Seco**†

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Introduction

Let $H = -\Delta + V$ be a Schrödinger operator on $\mathbb{R}^3$, and let E_k, $\varphi_k(x)$ be the eigenvalues and (normalized) eigenfunctions of H. We will study the eigenvalue sum and density, defined by

(1) $$\text{sneg}(H) = \sum_{E_k \le 0} E_k \ .$$

(2) $$\rho(x) = \sum_{E_k \le 0} |\varphi_k(x)|^2 \quad (x \in \mathbb{R}^3) \ .$$

The standard "semiclassical approximations" to these quantities are

(3) $$\text{sneg}(H) \approx -\frac{1}{15\pi^2} \int_{\mathbb{R}^3} \big(-V(x)\big)_+^{5/2} dx \ , \quad \text{and}$$

(4) $$\rho(x) \approx \frac{1}{6\pi^2} \big(-V(x)\big)_+^{3/2} \ .$$

(See [L].) Here, $t_+^s = t^s$ if $t > 0$, $t_+^s = 0$ if $t \le 0$.

In [FS1], we announced the proof of a precise asymptotic formula for the ground-state energy of a non-relativistic atom. To give the proof, one must understand and refine (3) and (4) for a particular radial potential V_{TF}^Z, the Thomas-Fermi potential for an atomic number Z. (See [L].) In [FS3], we reduced the asymptotic formula of [FS1] to the task of proving that

(5)
$$\text{sneg}(H) = -\frac{1}{15\pi^2} \int_{\mathbb{R}^3} \big(-V(x)\big)_+^{5/2} dx + \frac{Z^2}{8} + \frac{1}{48\pi^2} \int_{\mathbb{R}^3} \big(-V(x)\big)_+^{1/2} \Delta V dx + O(Z^{5/3-a})$$

and

(6)
$$\int\!\!\int_{\mathbb{R}^3 \times \mathbb{R}^3} \Big[\rho(x) - \frac{1}{6\pi^2} \big(-V(x)\big)_+^{3/2}\Big] \Big[\rho(y) - \frac{1}{6\pi^2} \big(-V(y)\big)_+^{3/2}\Big] \frac{dx dy}{|x-y|} = O(Z^{5/3-a})$$

for $V = V_{TF}^Z$, with $a > 0$ independent of Z.

Simpler and sharper reductions of [FS1] to (5) and (6) have been given by Bach [B], and by Graf-Solvej [GS]. The purpose of this paper is to prove (5) and (6), with $a = \frac{1}{150}$, for a class of radial potentials that includes V_{TF}^{Z}. This completes the proof of the results announced in [FS1].

Our proof of (5) and (6) is based on separation of variables. In [FS2, 4, 5] we made a careful study of ordinary differential operators. In [FS7], we used our ODE results to prove (6) for radial potentials V that satisfy a "non-resonance condition." The non-resonance condition is related to the scarcity of periodic orbits of a classical particle in the potential V. Here, we again use our results on ODE to show that (5) holds also, provided V satisfies another non-resonance condition, similar to that of [FS7]. Then we will show that the non-resonance conditions hold for a class of radial potentials including V_{TF}^{Z}. Our proof of the non-resonance condition uses elementary number theory, together with an inequality for the Thomas-Fermi potential proved in [FS6].

We believe that (5) and (6) can be proven for the Thomas-Fermi potential for a molecule, with errors $o(Z^{5/3})$. Moreover, we believe that the leading number-theoretic corrections to the density and eigenvalue sum for an atom can be computed rigorously. See Cordoba-Fefferman-Seco [CFS], as well as the introduction to [FS7].

We thank Maureen Schupsky for the skill and effort she has devoted to Texing our long, highly technical papers.

REVIEW OF EARLIER RESULTS

A. Eigenvalue Sums for Ordinary Differential Operators.

The results of this section are taken from [FS5].

I. The First WKB Eigenvalue Sum Theorem

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 $H = -\frac{d^2}{dx^2} + V(x)$ on I_{BVP}, with Dirichlet or Neumann boundary conditions; and let $\text{sneg}(H)$ be the sum of the negative eigenvalues of H. Our basic result on $\text{sneg}(H)$ is as follows.

First WKB Eigenvalue Sum Theorem.

$$\begin{aligned}\text{sneg}(H) = &-\frac{2}{3\pi}\int_{I_{\text{BVP}}} \big(-V(x)\big)_+^{3/2}\, dx + \frac{1}{24\pi}\int_{I_{\text{BVP}}} V''(x)\cdot\big(-V(x)\big)_+^{-1/2}\, dx \\ &+ \frac{\pi}{2}\big(\phi'(0)\big)^{-1}\tilde{\chi}\Big(\frac{1}{\pi}\phi(0) - \frac{1}{2}\Big) + \text{ Error }, \text{with} \\ &|\text{Error}| \le \Lambda^{5\varepsilon-2}|V(x_0)|\ .\end{aligned}$$

Here, $\phi(0) = \int_{I_{\text{BVP}}}\big(-V(x)\big)_+^{1/2}dx$, and $\phi'(0) = \frac{1}{2}\int_{I_{\text{BVP}}}\big(-V(x)\big)_+^{-1/2}dx$, and $\tilde{\chi}(t) = \min_{k\in\mathbb{Z}}|t-k-\frac{1}{2}|^2 - \frac{1}{12}$.

II. The Second WKB Eigenvalue Sum Theorem

Suppose we are given a smooth potential $V(x)$ defined on $(0,\infty)$, an interval $I \subset (0,\infty)$ containing $\{V(x) < 0\}$, and two positive functions $S(x)$, $B(x)$ defined on I. We will say that $V(x)$ has an *exact Coulomb singularity* with parameters (ℓ, E_0, Z, x_*) if the following conditions are satisfied:

(CS1) $V(x) = V_c(x) \equiv \frac{\ell(\ell+1)}{x^2} + E_0 - \frac{Z}{x}$ for $0 < x < 10x_*$

(CS2) $S(x) = \frac{Z}{x}$ and $B(x) = x$ for $x \in I$, $x < 10x_*$

(CS3) ℓ is an integer, and $0 \le \ell \le \frac{1}{16}(Zx_*)^{1/2}$

(CS4) $cZ^{4/3} < E_0 < CZ^{4/3}$

(CS5) $Z^{-\frac{98}{100}} < x_* < Z^{-\frac{1}{3}-\frac{1}{100}}$

(CS6) Z is greater than a large, positive constant determined by c and C in (CS4) above.

Strictly speaking, these conditions pertain to $V(x)$, $S(x)$, $B(x)$ rather than just $V(x)$, but this should cause no confusion.

Second WKB Eigenvalue Sum Theorem. *Suppose* $V(x)$ *is a smooth potential defined on* $(0,\infty)$, $I \subset (0,\infty)$ *is an interval containing* $\{V(x)<0\}$, *and* $S(x)$, $B(x)$ *are positive functions defined on* I. *Also, let* ε, K, N, ℓ, E_0, Z, x_* *be given.*

Assume the hypotheses (Z0)...(Z9) above, and assume that $V(x)$ *has an exact Coulomb singularity with parameters* (ℓ, E_0, Z, x_*). *(That is, assume (CS1)...(CS6)). Finally, suppose* $\ell > Z^{(10^{-9})}$.

Set $H = -\frac{d^2}{dx^2} + V(x)$ *on* $(0,\infty)$ *with Dirichlet boundary conditions. Then the sum of the negative eigenvalues of* H *is given by the equation*

$$\begin{aligned}
&\operatorname{sneg}(H) - \operatorname{sneg}(H_c) = \\
&\quad -\frac{2}{3\pi}\int_0^\infty \big(-V(x)\big)_+^{3/2} dx + \frac{1}{24\pi}\int_0^\infty V''(x)\cdot\big(-V(x)\big)_+^{-1/2} dx \\
&\quad + \frac{\pi}{2}\big(\phi'(0)\big)^{-1}\tilde{\chi}\Big(\frac{1}{\pi}\phi(0) - \frac{1}{2}\Big) + \frac{2}{3\pi}\int_0^\infty \big(-V_c(x)\big)_+^{3/2} dx \\
&\quad - \frac{1}{24\pi}\int_0^\infty V_c''(x)\cdot\big(-V_c(x)\big)_+^{-1/2} dx - \frac{2E_0^{3/2}}{Z}\tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}} - \sqrt{\ell(\ell+1)} - \frac{1}{2}\Big) \\
&\quad + \text{ Error },
\end{aligned}$$

with $H_c = -\frac{d^2}{dx^2} + V_c(x)$ *on* $(0,\infty)$ *subject to Dirichlet boundary conditions,* $V_c(x) = \frac{\ell(\ell+1)}{x^2} + E_0 - \frac{Z}{x}$, *and* $|\text{Error}| \le \Lambda^{5\varepsilon-2}\frac{Z}{x_*}$. *Recall that* $\phi(E) = \int_0^\infty \big(E - V(x)\big)_+^{1/2} dx$, $\phi'(E) = \frac{1}{2}\int_0^\infty \big(E - V(x)\big)_+^{-1/2} dx$, $\tilde{\chi}(t) = \min_{k\in\mathbb{Z}} |t - k - \frac{1}{2}|^2 - \frac{1}{12}$.

III. The Third WKB eigenvalue Sum Theorem

Let $\varepsilon, K, N > 0$ be given, with $\varepsilon N \ge 100$. Let $V(x)$ be a potential defined on a (possibly unbounded) interval I_{BVP}. Let S, B be positive numbers, and let $x_0 \in I_{\rm BVP}$ be given. Define $\lambda = S^{1/2}B$. Let E_∞ be a given energy, with $E_\infty > V(x_0)$. We make the following assumptions.

(H0*) $I = \{|x - x_0| < cB\} \subset I_{\rm BVP}$

(H1*) $|(\frac{d}{dx})^\alpha V(x)| \le C_\alpha S B^{-\alpha}$ in I

(H2*) $\frac{d^2}{dx^2} V \ge c' S B^{-2}$ in I

(H3*) $V'(x_0) = 0$

(H4*) For $x \in I_{\rm BVP} \backslash I$ we have $V(x) \ge \min\{E_\infty, V(x_0) + c''\lambda^{-2\varepsilon} S\}$.

(H5*) For $x \in I_{\rm BVP}$ with $|x - x_0| > \frac{1}{2}\lambda^K B$, we have $V(x) \ge E_\infty + \frac{1000}{|x - x_0|^2}$.

(H6*) λ is bounded below by a positive constant depending only on c, c', c'', C_α in (H0*)…(H4*), and on ε, K, N.

Third WKB Eigenvalue Sum Theorem. *Assume hypotheses (H0*)…(H6*) with $E_\infty = 0$, and assume also $-\lambda^{-3\varepsilon} S < V(x_0) < 0$. Then the sum of the negative eigenvalues of $H = -\frac{d^2}{dx^2} + V(x)$ on $I_{\rm BVP}$, with Dirichlet or Neumann boundary conditions, is given by*

$$sneg(H) = -\frac{2}{3\pi}\int_{I_{\rm BVP}} \big(-V(x)\big)_+^{3/2} dx + \frac{1}{24\pi}\int_{I_{\rm BVP}} V''(x)\cdot\big(-V(x)\big)_+^{-1/2} dx$$
$$+ \frac{\pi}{2}(\phi'(0))^{-1}\tilde{\chi}\Big(\frac{1}{\pi}\phi(0) - \frac{1}{2}\Big) + \text{ Error },$$

with $|\text{Error}| \le \lambda^{5\varepsilon - 2} S$.

Recall that $\phi(E) = \int_{I_{\rm BVP}} \big(E - V(x)\big)_+^{1/2} dx$, $\phi'(E) = \frac{1}{2}\int_{I_{\rm BVP}} \big(E - V(x)\big)_+^{-1/2} dx$, *and* $\tilde{\chi}(t) = \min_{k\in\mathbb{Z}} |t - k - \frac{1}{2}|^2 - \frac{1}{12}$.

IV. Eigenvalue Sums for Degenerate Potentials

The following results are taken from the section on degenerate potentials in [FS5].

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

Assumptions.

($\overline{Z0}$) 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 $|I| > cB(x)$.

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

($\overline{Z2}$) For $E_{\text{crit}} \leq E \leq 0$, the set $\{x \in I_{\text{BVP}} \mid V(x) \leq E\}$ 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 $\text{dist}\,(x_{\text{rt}}(E), \partial I) > cB(x_{\text{rt}}(E))$.

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

($\overline{Z4}$) For $E_{\text{crit}} \leq E \leq 0$, 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 $E_{\text{crit}} \leq E \leq 0$, we have $x_{\text{left}}(E) + cB(x_{\text{left}}(E)) \leq x_{\text{crit}}$.

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

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

($\overline{Z8}$) $\Lambda \equiv \left(\int_{x_{\text{left}}(0)}^{x_{\text{rt}}(0)} \frac{dx}{\lambda(x)B(x)}\right)^{-1}$ 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.

Theorem 1. *Suppose $V(x)$, $S(x)$, $B(x)$ satisfy hypotheses ($\overline{Z0}$)... ($\overline{Z8}$), and also suppose $V(x)$ has an exact Coulomb singularity (CS1)... (CS6) for a given (ℓ, E_0, Z, x_*). Assume $E_{\text{crit}} < -\frac{3Z}{x_*}$, with E_{crit} as in ($\overline{Z0}$)... ($\overline{Z8}$). Assume also $V(x) > -\frac{4}{3}\frac{Z}{x_*}$ for $x > x_*$. Set $V_c(x) = \frac{\ell(\ell+1)}{x^2} + E_0 - \frac{Z}{x}$. Then for $H = -\frac{d^2}{dx^2} + V(x)$, $H_c = -\frac{d^2}{dx^2} + V_c(x)$ on $(0, \infty)$ with Dirichlet boundary conditions, we have*

$$sneg(H) - sneg(H_c) = -\frac{2}{3\pi}\int_0^\infty \left\{\big(-V(x)\big)_+^{3/2} - \big(-V_c(x)\big)_+^{3/2}\right\} dx + \text{ Error },$$

with $|\text{Error}| < C\frac{Z}{x_*}$. *Here,* C *depends only on the constants in* ($\bar{Z0}$)...($\bar{Z8}$) *and in (CS1)...(CS6).*

β. *Set-Up.*

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

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

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.

In addition to (1), we make the following assumptions.

Hypotheses.

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

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

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

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

($\hat{Z4}$) For $x \in (0, x_{\text{small}}]$ we have $V(x) \ge \underline{c}x_0^{-2}$

($\hat{Z5}$) For $x \in [x_{\text{small}}, x_0]$ we have $|V(x)| \le \underline{C}x_0^{-2}$

($\hat{Z6}$) We have $x_{\text{big}} < \underline{C}x_1$ and $V(x)$ is increasing in $[x_1, x_{\text{big}}]$.

($\hat{Z7}$) For $x \in \left[\frac{x_1}{8}, x_{\text{big}}\right]$, we have $|V(x)| \le \underline{C}x_1^{-2}$.

($\hat{Z8}$) For $x \in [x_{\text{big}}, \infty)$, we have $V(x) \ge 0$.

($\hat{Z9}$) For $E \in [V(x_*), 0]$ we have
$\int_{x_0}^{x_{\text{crit}}} \left(E - V(x)\right)^{-1/2} dx \le \delta \cdot \int_{x_0}^{\frac{1}{2}x_*} \left(E - V(x)\right)^{-1/2} dx.$

Theorem 2. *Suppose* $V(x)$, $S(x)$, $B(x)$ *satisfy hypotheses* ($\hat{Z0}$)...($\hat{Z9}$), *and suppose also that* $V(x)$ *has an exact Coulomb singularity (CS1)...(CS6) for a given*

(ℓ, E_0, Z, x_*). Assume $V(x) > -\frac{2Z}{x_*}$ for $x > x_*$. Assume $V(2x_0) < -\frac{8Z}{x_*}$, and assume

$$(1) \qquad \int_0^\infty \{ (-V(x))_+^{1/2} - (V(\tfrac{1}{2}x_1) - V(x))_+^{1/2} \} dx < \underline{C} \, ,$$

where x_0, x_1 are as in $(\hat{Z0}) \ldots (\hat{Z9})$. Set $V_c(x) = \frac{\ell(\ell+1)}{x^2} + E_0 - \frac{Z}{x}$. Then for $H = -\frac{d^2}{dx^2} + V(x)$, $H_c = -\frac{d^2}{dx^2} + V_c(x)$ on $(0, \infty)$ with Dirichlet boundary conditions, we have

$$sneg(H) - sneg(H_c) = -\frac{2}{3\pi} \int_0^\infty \{ (-V(x))_+^{3/2} - (-V_c(x))_+^{3/2} \} dx + \text{ Error } ,$$

with $|\text{Error}| < C\frac{Z}{x_*}$. Here C depends only on $\underline{C}$ in (1), and on the constants in $(\hat{Z0}) \ldots (\hat{Z9})$ and in (CS1)...(CS6).

γ**.** *Set-up.* 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

$$(1) \qquad 16x_0 < x_{\text{crit}} \, , \; 16x_{\text{crit}} < \frac{1}{10}x_* \, , \; \frac{16}{10}x_* < x_1 \, , \; 16x_1 < x_{\text{big}} \, .$$

In addition to (1), we make the following assumptions.

Hypotheses.

- $(Z0^\dagger)$ If $x, y \in I$ and $|x - y| < \frac{1}{2}B(x)$, then $c < S(y)/S(x) < C$.
- $(Z1^\dagger)$ If $x \in I$ and $\alpha \geq 0$, then $\left| \left(\frac{d}{dx}\right)^\alpha V(x) \right| \leq C_\alpha S(x) B^{-\alpha}(x)$.
- $(Z2^\dagger)$ If $x \in I$, then $V(x) < -cS(x)$ and $V'(x) > cS(x)B^{-1}(x)$.
- $(Z3^\dagger)$ $\Lambda = \left(\int_I \frac{dx}{\lambda(x)B(x)} \right)^{-1}$ is greater than a certain large, positive number determined by c, C, C_α in $(Z0^\dagger) \ldots (Z2^\dagger)$.
- $(Z4^\dagger)$ $|V(x)| \leq \underline{C}/(x_0 x)$ for $x \in (0, x_0]$.
- $(Z5^\dagger)$ $V(x)$ 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 $E \in [V(\frac{x_*}{10}), 0]$, we have

$$\int_{x_0}^{x_{\text{crit}}} \big(E - V(x)\big)^{-1/2} dx \leq \delta \cdot \int_{x_0}^{\frac{1}{20}x_*} \big(E - V(x)\big)^{-1/2} dx.$$

Theorem 3. *Suppose $V(x)$, $S(x)$, $B(x)$ satisfy hypotheses (Z0†)...(Z7†). Suppose also that $V(x)$ has an exact Coulomb singularity (CS1)...(CS6) for given (ℓ, E_0, Z, x_*). [We take the same x_* in (Z0†)... (Z7†) as in (CS1)...(CS6)]. We make the following additional assumptions:*

$$V\Big(\frac{x_*}{10}\Big) < -\frac{3Z}{x_*} \tag{2}$$

$$V(x) > -\frac{4}{3}\,\frac{Z}{x_*} \quad \textit{for} \quad x > x_* \tag{3}$$

$$V(x) > -Cx_{\text{big}}^2 x^{-4} \quad \textit{for } x > x_{\text{big}} \ . \tag{4}$$

$$\int_0^\infty \big\{\big(-V(x)\big)_+^{1/2} - \big(V(\tfrac{1}{4}x_1) - V(x)\big)_+^{1/2}\big\} dx < \underline{C} \ , \tag{5}$$

with x_1 as in (Z0†)...(Z7†).

Set $V_c(x) = \frac{\ell(\ell+1)}{x^2} + E_0 - \frac{Z}{x}$. Then for $H = -\frac{d^2}{dx^2} + V(x)$, $H_c = -\frac{d^2}{dx^2} + V_c(x)$ on $(0, \infty)$ with Dirichlet boundary conditions, we have

$$\text{sneg}(H) - \text{sneg}(H_c) = -\frac{2}{3\pi} \int_0^\infty \big\{\big(-V(x)\big)_+^{3/2} - \big(-V_c(x)\big)_+^{3/2}\big\} dx + \text{ Error } ,$$

with $|\text{Error}| < \frac{CZ}{x_*}$. Here, C depends only on $\underline{C}$ in (5), and on the constants in (Z0†)...(Z7†), (CS1)...(CS6), and (4).

B. Approximate Thomas-Fermi Potentials.

The following results are taken from the section on the Density in an Approximate Thomas-Fermi Potential in [FS7].

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 $V_Z^{TF}(r) = -\frac{Z}{r} + O(Z^{4/3})$ as $r \to 0+$.

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

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

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

Specifically, we have

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

(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

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

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

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 eigenvalue sum 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 eigenvalue sums, 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 $\Omega(\Omega+1) = \max_{r>0}\big(-r^2V(r)\big)$, 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 $x_{\text{left}}(\ell)$, $x_0(\ell)$, $x_{\text{rt}}(\ell)$:

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

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

Moreover,

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

$$c_1<1/2\ . \tag{13b}$$

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, $0<c_2<1/2$.

Using the properties (3)...(15) of $V_\ell(r)$, we can verify the hypotheses of our results from section A.IV above, on the eigenvalue sum. 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 $\ell=0$, the potential $V_\ell(r)$ satisfies hypotheses (Z0†)...(Z7†) of Theorem 3 in section A.IVα above, 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 constant, determined* *by the C_α in (1). Then for $Z^{10^{-9}} \geq \ell \geq 1$, the potential $V_\ell(r)$ satisfies hypotheses $(\hat{Z0})\dots(\hat{Z9})$ of Theorem 2 in section A.IVβ above, with the weight functions $S(r)$ as in (0), $B(r) \equiv r$. The constants in $(\hat{Z0})\dots(\hat{Z9})$ depend only on ℓ and on the C_α in (1).*

Remark. Since the constants in $(\hat{Z0})\dots(\hat{Z9})$ 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 $(\overline{Z0})\dots(\overline{Z8})$ of Theorem 1 in section A.IVα above, with the weight functions $S(r)$ as in (0), $B(r) \equiv r$. The constants in $(\overline{Z0})\dots(\overline{Z8})$ 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 First WKB Eigenvalue Sum Theorem, 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 First WKB Eigenvalue Sum Theorem. 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 $|\min V_\ell| \sim \tilde{S}$, $V_\ell'' \sim \tilde{S}\tilde{B}^{-2}$ 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 the hypotheses of the Third WKB Eigenvalue Sum Theorem, with* $\lambda \sim S^{1/2}(\check{r})\check{r} \sim \Omega$*. The constants in the hypotheses (H0*)…(H6*) depend only on* ε*,* N *and the* C_α *in (1).*

Remark. The version of Lemma 6 stated in [FS7] trivially implies the version stated here.

We shall also need to understand the function

$$W(r) = -r^2 V(r) \tag{16}$$

when V is an approximate T-F potential. Set

$$\mathcal{S}(r) = r^2 S(r) = \min\{Zr, r^{-2}\} \quad \text{for } r > 0 \ . \tag{17}$$

Then we have the following result.

Lemma 7. *The function* $W(r)$ *satisfies*

$$\left|\left(\frac{d}{dr}\right)^\alpha W(r)\right| \le C_\alpha \mathcal{S}(r) r^{-\alpha} \quad \textit{for } r > 0 \ , \ \alpha \ge 0 \ . \tag{18}$$

Moreover, $W(r)$ *has a single critical point* $r = \check{r}$*, at which we have*

$$cZ^{-1/3} < \check{r} < CZ^{-1/3} \quad \textit{and} \tag{19}$$

$$(20) \qquad -W''(\check{r}) > c\mathcal{S}(\check{r})(\check{r})^{-2} \ .$$

Given any $c_1 > 0$ we can find $c_2 > 0$ depending on c_1 such that

$$(21) \qquad |W'(r)| > c_2\mathcal{S}(r)r^{-1} \quad \textit{for } |r-\check{r}| > c_1\check{r} \ .$$

Sketch of Proof. Estimates (18) follow at once from (i) above. When $V = V_{TF}$, the estimates (19), (20), (21) follow by rescaling from the case $Z = 1$, which in turn follows from the section on Elementary Properties of the TF Potential in [FS7]. Hence, (19), (20) and (21) hold for any V that satisfies (2). Details are left to the reader. ■

We close this section by noting that the Thomas-Fermi potential satisfies

$$(22) \quad \left|\left(\frac{d}{dr}\right)^\alpha\left\{E_0 - \frac{Z}{r} - V_{TF}^Z(r)\right\}\right| \le C_\alpha Z^{3/2}r^{1/2-\alpha} \text{for } \alpha \ge 0 \text{ and } 0 < r < cZ^{-1/3} \ ,$$

with a constant E_0 satisfying

$$(23) \qquad cZ^{4/3} < E_0 < CZ^{4/3} \ .$$

These standard estimates follow, e.g. from Lemma 1 in the section on Elementary Properties of the Thomas-Fermi Potential in [FS7].

C. The Density in an Approximate T-F Potential.

The following are the main results of [FS7].

Let $V_Z^{\rm TF}(x)$ be the Thomas-Fermi potential on $\mathbb{R}^3$. Thus $-\Delta V_Z^{\rm TF} = (\text{const.})|V_Z^{\rm TF}|^{3/2}$ on $\mathbb{R}^3\backslash\{0\}$, and

$$V_Z^{TF}(x) = -\frac{Z}{|x|} + O(Z^{4/3}) \quad \text{as } x \to 0 \ .$$

Let $V(x)$ be a radially symmetric potential on $\mathbb{R}^3$. We write also $V(r)$, $V_Z^{\rm TF}(r)$ as functions of one variable. Assume

$$(1) \qquad \left|\left(\frac{d}{dr}\right)^\alpha V(r)\right| \le C_\alpha r^{-\alpha}\min\left\{\frac{Z}{r}, r^{-4}\right\} \quad \text{for } \alpha \ge 0 \ ,$$

$$(2) \qquad \Big|\Big(\frac{d}{dr}\Big)^{\alpha}\{V(r) - V_Z^{\mathrm{TF}}(r)\}\Big| \le c_0 r^{-\alpha} \min\Big\{\frac{Z}{r}, r^{-4}\Big\} \quad \text{for } 0 \le \alpha \le 2\ ,$$

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 $|U(x)| \le C$, $|\nabla U(x)| \le C\delta^{-1}$. Assume Z is greater than a certain large, positive constant determined by the C_α in (1).*

Then

$$\Big|\int_{\mathbb{R}^3} U(x)\rho_{\mathrm{error}}(x)dx\Big| \le C'Z\delta + C'Z^{\frac{1}{3}+2\cdot 10^{-9}}\ .$$

The constant C' depends only on C above, and on the C_α in (1).

For a more refined estimate, we introduce Ω, the positive root $\Omega(\Omega+1) = \max_{r>0}\big(-r^2V(r)\big)$. 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 $\int_{\mathbb{R}^3 \times \mathbb{R}^3} \rho_{\text{error}}(x) \rho_{\text{error}}(y) \frac{dxdy}{|x-y|} \le C' Z^{\frac{5}{3} - \frac{2}{3}a}$. *The constant* C' *depends only on* C, a *and the* C_α *in (1).*

D. Approximating Sums by Integrals.

The following lemma is taken from [FS4]. For real numbers t, define:

$$\chi_+(t) = k - t - \frac{1}{2} \quad \text{for } k \text{ the smallest integer } \ge t \ ;$$
$$\chi_-(t) = t - k - \frac{1}{2} \quad \text{for } k \text{ the largest integer } \le t \ ;$$
$$\tilde{\chi}(t) = \min_{k \in \mathbb{Z}} |t - k - \frac{1}{2}|^2 - \frac{1}{12} \ .$$

Lemma on Riemann Sums. *Let* $f(t)$, $\sigma(t)$, $\tau(t)$ *be defined on a non–empty interval* $[a,b]$. *Suppose* $\sigma(t) > 0$, $\tau(t) \ge 1$ *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* $|(\frac{d}{dt})^m f(t)| \le C_m \sigma(t) \tau^{-m}(t)$ *for* $t \in [a,b]$. *Then* $\sum_{k \in \mathbb{Z} \cap [a,b]} f(k) = \int_a^b f(t)dt - f(b)\chi_-(b) - f(a)\chi_+(a) + \frac{1}{2} f'(b)\tilde{\chi}(b) - \frac{1}{2} f'(a)\tilde{\chi}(a) + \text{Error}$ *with* $|\text{Error}| \le C'\sigma(a)\tau^{-2}(a) + C'\sigma(b)\tau^{-2}(b) + C'_N \int_a^b \sigma(t)\tau^{-N}(t)dt$. *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* $|\text{Error}| \le C'\sigma(b)\tau^{-2}(b) + C'_N \int_a^b \sigma(t)\tau^{-N}(t)dt$, *with* C', C'_N *as before. Similarly, if* $f(t) = 0$ *to infinite order at* $t = b$, *then* $|\text{Error}| \le C'\sigma(a)\tau^{-2}(a) + C'_N \int_a^b \sigma(t)\tau^{-N}(t)dt$. *If* $f(t) = 0$ *to infinite order at both* $t = a$ *and* $t = b$, *then* $|\text{Error}| \le C'_N \int_a^b \sigma(t)\tau^{-N}(t)dt$.

E. An Auxiliary Function Arising from the Thomas-Fermi Potential.

Let $V_{TF}^{Z}(r)$ be the Thomas-Fermi potential, and let $t_{\max} = \sup_{r>0}\big[-r^2 V_{TF}^{Z}(r)\big]^{1/2}$. For $0 < t < t_{\max}$, define $\Theta(t) = \int_0^\infty \big(-V_{TF}^{Z}(r) - \frac{t^2}{r^2}\big)_+^{1/2} dr$. The following inequality is equivalent by a trivial rescaling to the main result of [FS6].

Theorem. $\left|\frac{d^2}{dt^2}\Theta(t)\right| \geq cZ^{-1/3}$ *for* $0 < t < t_{\max}$*, with* $c > 0$ *independent of* t *and* Z*.*

F. Elementary Integrals.

The following elementary identities come from [FS5].

Lemma 1. *Let* $V_c^{\ell}(r) = \frac{\ell(\ell+1)}{r^2} + E_0 - \frac{Z}{r}$*, and define*

$$n_\ell = \int_0^\infty \big(-V_c^{\ell}(r)\big)_+^{-1/2} dr \ , \ \phi_\ell = \frac{1}{\pi}\int_0^\infty \big(-V_c^{\ell}(r)\big)_+^{1/2} dr - \frac{1}{2} \ .$$

Then $\frac{\pi}{n_\ell}\tilde{\chi}(\phi_\ell) = \frac{2E_0^{3/2}}{Z}\tilde{\chi}\big(\frac{Z}{2E_0^{1/2}} - \sqrt{\ell(\ell+1)} - \frac{1}{2}\big)$*.*

(See the paragraph just before the statement of the second WKB eigenvalue sum theorem in [FS5].)

Lemma 2. *If* Q*,* A*,* P*,* $Q^2 - 4AP > 0$*, then*

$$\frac{1}{\pi}\int_0^\infty \big(-(\frac{P}{t^2} - \frac{Q}{t} + A)\big)_+^{1/2} dt = \frac{Q}{2\sqrt{A}} - \sqrt{P} \ .$$

(See equation (10) in the section of [FS5] on the second WKB eigenvalue sum theorem).

The Eigenvalue Sum for an Approximate TF Potential with an Exact Coulomb Singularity

Let $V(r)$ be a potential on $(0,\infty)$, which approximates the T-F potential $V_Z^{TF}(r)$ in the following sense.

(1) $$\Big|\big(\frac{d}{dr}\big)^\alpha V(r)\Big| \le C_\alpha r^{-\alpha}\min\{\frac{Z}{r}, r^{-4}\}, \quad \text{all } r\in(0,\infty), \alpha\ge 0\ .$$

(2) $$\Big|\big(\frac{d}{dr}\big)^\alpha\{V(r)-V_Z^{TF}(r)\}\Big| \le c_0 r^{-\alpha}\min\{\frac{Z}{r}, r^{-4}\} \quad \text{for } 0\le\alpha\le 2 \text{ and all } r\ .$$

Here c_0 is a small constant determined by the C_α in (1).

(3) For $0<r<Z^{2\varepsilon-3/5}$ we have $V(r)=E_0-\dfrac{Z}{r}$, with $cZ^{4/3}<E_0<CZ^{4/3}$.

If (1), (2), (3) hold, then we say $V(r)$ is an "approximate TF potential with an exact Coulomb singularity."

We assume also that Z is greater than a certain large positive constant determined by ε, c, C in (3), and by the C_α in (1).

Our goal is to compute the sum sneg (H) of the negative eigenvalues of $H=-\Delta+V(|x|)$ on $\mathbb{R}^3$ for an approximate TF potential with an exact Coulomb singularity. In a later section, we will remove assumption (3) by using perturbation theory.

Separation of variables gives

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

(5)
$$H_\ell=-\frac{d^2}{dr^2}+V_\ell(r)\equiv-\frac{d^2}{dr^2}+\Big(\frac{\ell(\ell+1)}{r^2}+V(r)\Big)\text{on } (0,\infty) \text{ (Dirichlet boundary conditions)}\ .$$

Introduce for comparison $V_\ell^c(r)=\frac{\ell(\ell+1)}{r^2}+E_0-\frac{Z}{r}$ and $H_\ell^c=-\frac{d^2}{dr^2}+V_\ell^c(r)$ on $(0,\infty)$.

Define Ω to be the positive root of $\Omega(\Omega+1) = \max_{r>0}\big(-r^2V(r)\big)$, and suppose the maximum is attained at $\check{r}$. Thus $\Omega \sim Z^{1/3}$, $\check{r} \sim Z^{-1/3}$. Similarly, define Ω_c to be the positive root of $\Omega_c(\Omega_c+1) = \max_{r>0}\big(-r^2V_c(r)\big)$, with $V_c(r) = E_0 - \frac{Z}{r}$, and suppose the maximum is attained at $\check{r}_c$. Thus, $\Omega_c \sim Z^{1/3}$ and $\check{r}_c \sim Z^{-1/3}$.
For $\ell \geq \Omega$ we have $V_\ell(r) \geq 0$ everywhere, so $\text{sneg}\,(H_\ell) = 0$. Similarly, for $\ell \geq \Omega_c$ we have $\text{sneg}\,(H_\ell^c) = 0$.

Note that for $0 \leq \ell \leq Z^{+1/5}$ and $x_* \sim Z^{\varepsilon-3/5}$, the potential $V_\ell(r)$ satisfies conditions (CS1)...(CS6) with any $I \subset (0,\infty)$ containing $\{V_\ell < 0\}$, with $S(r) = \min\{\frac{Z}{r}, r^{-4}\}$ and $B(r) = r$, and with parameters (ℓ, E_0, Z, x_*). (Conditions (CS1)...(CS6) appear in the section on the second eigenvalue sum theorem.) In fact, (CS1) follows from (3); (CS2) follows from the definition of $S(r)$, $B(r)$; (CS3) holds since $0 \leq \ell \leq Z^{1/5} \leq \frac{1}{16}(Z \cdot cZ^{\varepsilon-3/5})^{1/2}$; (CS4) is contained in (3); (CS5) is immediate from $x_* \sim Z^{\varepsilon-3/5}$; and (CS6) is contained in our assumption that Z exceeds a large constant determined by ε, c, C in (3) and C_α in (1).

Our plan is to use our theorems on the eigenvalue sum of an ODE to compute $\text{sneg}\,(H_\ell) - \text{sneg}\,(H_\ell^c)$, and then to substitute the results into (4), (5).

The following quantities, familiar from the discussion of the three-dimensional density, will play a role here as well:

$$(6) \qquad \phi_\ell = \frac{1}{\pi}\int_0^\infty \big(-V_\ell(r)\big)_+^{1/2} dr - \frac{1}{2} = \frac{1}{\pi}\int_0^\infty \Big(-\frac{\ell(\ell+1)}{r^2} - V(r)\Big)_+^{1/2} dr - \frac{1}{2}$$

$$(7) \qquad n_\ell = \int_0^\infty \big(-V_\ell(r)\big)_+^{-1/2} dr = \int_0^\infty \Big(-\frac{\ell(\ell+1)}{r^2} - V(r)\Big)_+^{-1/2} dr\ .$$

Let us begin computing $\text{sneg}\,(H_\ell) - \text{sneg}(H_\ell^c)$.

Lemma 1. *Set* $x_0 = \overline{C}Z^{-1}$, $x_{\text{crit}} = Z^{-9/10}$ $x_* = Z^{\varepsilon-3/5}$, $x_1 = 1/\overline{C}$, $x_{\text{big}} = \overline{C}$, $\delta = \overline{C}Z^{-3/20}$ *with* $\overline{C}$ *a large constant depending on* ε, c, C, C_α *in (1)...(3). Then for* $\ell = 0$, *the potential* $V_\ell(r)$ *satisfies the hypotheses of Theorem 3 in the section on Eigenvalue Sums in Degenerate Potentials.*

Proof. By Lemma 1 of the section on Approximate TF Potentials, $V(r)$ satisfies $(\mathrm{Z0}^\dagger)\ldots(\mathrm{Z7}^\dagger)$ with x_* replaced by $x_*^{\mathrm{old}} =$ (const.) $Z^{-8/10}$. (See section A.IVγ for conditions $(\mathrm{Z0}^\dagger)\ldots(\mathrm{Z7}^\dagger)$.) Now, x_* enters $(\mathrm{Z0}^\dagger)\ldots(\mathrm{Z7}^\dagger)$ only in $(\mathrm{Z7}^\dagger)$. Moreover, $x_*^{\mathrm{old}} < x_*$ and $V(x_*^{\mathrm{old}}) < V(x_*)$. (Recall that V is increasing since $(V_Z^{TF})' > cr^{-1}\min\{\frac{Z}{r}, r^{-4}\}$ and $|V' - (V_Z^{TF})'| \leq c_0 r^{-1}\min\{\frac{Z}{r}, r^{-4}\}$.) Hence $(\mathrm{Z7}^\dagger)$ for x_*^{old} implies $(\mathrm{Z7}^\dagger)$ for x_*. Thus $(\mathrm{Z0}^\dagger)\ldots(\mathrm{Z7}^\dagger)$ hold for our present x_0, x_{crit}, x_*, x_1, x_{big}, δ. With $I = (0,\infty)$, conditions (CS1)…(CS6) hold also, since $\ell = 0 < Z^{1/5}$. Aside from $(\mathrm{Z0}^\dagger)\ldots(\mathrm{Z7}^\dagger)$ and (CS1)…(CS6), the remaining hypotheses of Theorem 3 on Eigenvalue Sums in Degenerate Potentials are as follows:

$$V\left(\frac{x_*}{10}\right) < -\frac{3Z}{x_*} \tag{8}$$

$$V(x) > -\frac{4}{3}\frac{Z}{x_*} \quad \text{for } x > x_* \tag{9}$$

$$\int_0^\infty \left\{\left(-V(x)\right)_+^{1/2} - \left(V(\tfrac{1}{4}x_1) - V(x)\right)_+^{1/2}\right\}dx \leq \underline{C}\,. \tag{10}$$

$$V(x) > -Cx_{\mathrm{big}}^2 x^{-4} \quad \text{for } x > x_{\mathrm{big}}\,. \tag{10a}$$

To verify these conditions, recall that

$$|V_{TF}^Z(r) + \frac{Z}{r} - E_0| < \bar{\bar{c}}Z^{4/3}(Z^{1/3}r)^{1/2} \quad \text{for } r < Z^{-1/3}$$

and $V_{TF}^Z(r) > -\frac{Z}{r}$ for all r.

Therefore for $x_* = Z^{\varepsilon - 3/5}$, we have from (2) that $\left|V(\frac{x_*}{10}) + \frac{Z}{(x_*/10)}\right| < 2c_0\frac{Z}{(x_*/10)}$, so (8) is obvious. Also from (2), $V(r) \geq -(1+c_0)\frac{Z}{r}$ for all r, so (9) is obvious. Since $x_1 = 1/\overline{C}$, (1), (2) show that $V(\frac{1}{4}x_1) < 0$ and $|V(\frac{1}{4}x_1)| \leq \underline{C}$. Hence

$$\left|\left(-V(x)\right)_+^{1/2} - \left(V(\frac{1}{4}x_1) - V(x)\right)_+^{1/2}\right| \leq \begin{cases} C\left(-V(x)\right)^{-1/2} & \text{if } -V(x) > \underline{C} \\ C\left(-V(x)\right)^{+1/2} & \text{if } -V(x) \leq \underline{C} \end{cases}.$$

Since $-V(x) \sim \min\{\frac{Z}{r}, r^{-4}\}$ by (1), (2), it follows that

$$\left|\left(-V(r)\right)_+^{1/2} - \left(V(\tfrac{1}{2}x_1) - V(r)\right)_+^{1/2}\right| \le \begin{cases} C\left(\min\{\frac{Z}{r}, r^{-4}\}\right)^{-1/2} \le C' & \text{if } 0 < r < 1 \\ C(r^{-4})^{+1/2} = Cr^{-2} & \text{if } 1 < r < \infty \end{cases}$$

so (10) is obvious. Finally, (10a) follows from (1), (2) since $x_{\text{big}} = \overline{C}$. The proof of the lemma is complete. ■

By Lemma 1 above, and Theorem 3 in the section on Eigenvalue Sums for Degenerate Potentials, we have

$$\text{(11)} \quad \operatorname{sneg}(H_\ell) - \operatorname{sneg}(H_\ell^c) = -\frac{2}{3\pi}\int_0^\infty \left\{\left(-V_\ell(x)\right)_+^{3/2} - \left(-V_\ell^c(x)\right)_+^{3/2}\right\}dx + \text{ Err}_0$$

when $\ell = 0$, where

$$\text{(12)} \qquad |\text{Err}_0| \le C\frac{Z}{x_*} = CZ^{-\varepsilon+8/5} .$$

Lemma 2. *Set* $x_0 = \overline{C}\ell^2 Z^{-1}$, $x_{\text{crit}} = Z^{-9/10}$, $x_* = Z^{\varepsilon-3/5}$, $x_{\text{small}} = \ell^2/(\overline{C}Z)$, $x_1 = 1/(\overline{C}\ell)$, $x_{\text{big}} = (1+c_1)x_{\text{rt}}(\ell)$, $\delta = \overline{C}Z^{-3/20}$, *with* $\overline{C}$ *a large constant determined by the* C_α *in (1). Then for* $1 \le \ell \le Z^{10^{-9}}$, *the potential* $V_\ell(r)$ *satisfies the hypotheses of Theorem 2 in the section on Eigenvalue Sums for Degenerate Potentials, with constants depending on* ℓ.

Remarks. For the definition of $x_{\text{rt}}(\ell)$, see equations (3)...(15) in the section on Approximate TF Potentials. Note that we can use Lemma 2 only for $1 \le \ell \le$ (Large Constant), since the conclusion of the Lemma involves constants depending on ℓ.

Proof of Lemma 2. We know that conditions $(\text{Z}\hat{0})\ldots(\text{Z}\hat{9})$ hold for $V_\ell(r)$, with constants depending on ℓ, and with x_* replaced by $x_*^{\text{old}} = Z^{-8/10}$. That follows from Lemma 2 in the section on Approximate TF Potentials. (For conditions $(\text{Z}\hat{0})\ldots(\text{Z}\hat{9})$, see section A.IV$\beta$.)

Now, x_* enters $(\mathrm{Z}\hat{0})\dots(\mathrm{Z}\hat{9})$ only in $(\mathrm{Z}\hat{9})$. Moreover, $(\mathrm{Z}\hat{9})$ for x_*^{old} implies $(\mathrm{Z}\hat{9})$ for x_*, provided $x_*^{\mathrm{old}} < x_*$ and $V_\ell(x_*{}^{\mathrm{old}}) < V_\ell(x_*)$. Let us check these conditions. Certainly $x_*^{\mathrm{old}} < x_*$, by definition. Also, $-V(r) \sim \min\{\frac{Z}{r}, r^{-4}\}$ by (1), (2); and $V_\ell(r) = \frac{\ell(\ell+1)}{r^2} + V(r)$; and $\frac{\ell(\ell+1)}{r^2} << \min\{\frac{Z}{r}, r^{-4}\}$ when $r = x_*$ or $r = x_*^{\mathrm{old}}$, $\ell \le Z^{10^{-9}}$. Therefore, $-V_\ell(r) \sim \min\{\frac{Z}{r}, r^{-4}\}$ for $r = x_*$ and for $r = x_*^{\mathrm{old}}$. It follows that $-V_\ell(x_*) < -V_\ell(x_*^{\mathrm{old}})$, i.e. $V_\ell(x_*^{\mathrm{old}}) < V_\ell(x_*)$ as asserted above. Thus, $(\mathrm{Z}\hat{0})\dots(\mathrm{Z}\hat{9})$ hold. Also (CS1)... (CS6) hold with $I = (0,\infty)$, since $\ell \le Z^{1/5}$ here. Aside from $(\mathrm{Z}\hat{0})\dots(\mathrm{Z}\hat{9})$, (CS1)...(CS6), the only remaining hypotheses of Theorem 2 in the section on Eigenvalue Sums in Degenerate Potentials are the following.

(13) $$V_\ell(x) > -\frac{2Z}{x_*} \quad \text{for } x > x_*$$

(14) $$V_\ell(2x_0) < -\frac{8Z}{x_*}$$

(15) $$\int_0^\infty \{\left(-V_\ell(x)\right)_+^{1/2} - \left(V_\ell(\frac{1}{2}x_1) - V_\ell(x)\right)_+^{1/2}\}dx \le \underline{C}\ ,$$

with $\underline{C}$ allowed to depend on ℓ .

Recall that $V(x) \ge -(1+c_0)\frac{Z}{x}$ for all x, and that $\frac{\ell(\ell+1)}{x_0^2} \le 2(\overline{C})^{-1}\frac{Z}{x_0}$ by definition of x_0. Hence for $x > x_*$ we have $V_\ell(x) > V(x) > -\frac{2Z}{x} > -\frac{2Z}{x_*}$, which proves (13). Also

$$V_\ell(2x_0) \le 2(\overline{C})^{-1}\frac{Z}{x_0} + V(2x_0) \le \left\{2(\overline{C})^{-1} + c_0\right\}\frac{Z}{x_0} + V_Z^{TF}(2x_0)\ .$$

Since $2x_0 << Z^{-1/3}$, we have $V_Z^{TF}(2x_0) \le -(1-c_0)\frac{Z}{2x_0}$, so $V_\ell(2x_0) \le \{2(\overline{C})^{-1} + c_0 - \frac{(1-c_0)}{2}\}\frac{Z}{x_0} < -\frac{8Z}{x_*}$ because $x_* >> x_0$. This proves (14).

We control $V_\ell(r)$ by equations (3)...(15) in the section on Approximate TF Potentials. From those equations, we recall that

$$\{V_\ell(r) < 0\} = (x_{\mathrm{left}}(\ell), x_{\mathrm{rt}}(\ell)) \text{ with } x_{\mathrm{left}}(\ell) \sim \frac{\ell^2}{Z}\ , x_{\mathrm{rt}}(\ell) \sim \frac{1}{\ell}\ ,$$

and that $|V_\ell(r)| \le C\min\{\frac{Z}{r}, r^{-4}\}$ in $[x_{\rm left}(\ell), x_{\rm rt}(\ell)]$. Since $x_1 = \frac{1}{\overline{C}\ell}$ and $1 \le \ell \le Z^{10^{-9}}$, we have $\frac{1}{2}x_1 \in [x_{\rm left}(\ell), x_{\rm rt}(\ell)]$, so $0 \le -V_\ell(\frac{1}{2}x_1) \le C(\overline{C}\ell)^4$. This implies

$$0 \le \left\{ \left(-V_\ell(r)\right)_+^{1/2} - \left(V_\ell(\frac{1}{2}x_1) - V_\ell(r)\right)_+^{1/2} \right\} \le \begin{cases} C(\overline{C}\ell)^4\left(-V_\ell(r)\right)^{-1/2} & \text{if } -V_\ell(r) > (\overline{C}\ell)^4 \\ C(\overline{C}\ell)^{4/2} & \text{if } 0 < -V_\ell(r) \le (\overline{C}\ell)^4 \\ 0 & \text{if } -V_\ell(r) < 0 \ . \end{cases}$$

Hence

$$0 \le \left\{ \left(-V_\ell(r)\right)_+^{1/2} - \left(V_\ell(\frac{1}{2}x_1) - V_\ell(r)\right)_+^{1/2} \right\} \le (\text{Const.})\ell^2 \chi_{r\in[x_{\rm left}(\ell), x_{\rm rt}(\ell)]} \ ,$$

which makes (15) obvious. The proof of Lemma 2 is complete. ■

¿From Lemma 2 above, and from Theorem 2 in the section on Eigenvalue Sums for Degenerate Potentials, we conclude that

$$\text{(16)} \quad \text{sneg}(H_\ell) - \text{sneg}(H_\ell^c) = -\frac{2}{3\pi}\int_0^\infty \left\{ \left(-V_\ell(r)\right)_+^{3/2} - \left(-V_\ell^c(r)\right)_+^{3/2} \right\} dr + \text{Err}_\ell$$

for $1 \le \ell \le Z^{10^{-9}}$, with

$$\text{(17)} \qquad |\text{Err}_\ell| \le C(\ell)\frac{Z}{x_*} = C(\ell) Z^{-\varepsilon+8/5} \ .$$

Lemma 3. *Pick I, $x_{\rm crit}$, $E_{\rm crit}$, δ as in Lemma 3 in the section on Approximate TF Potentials, and let $\overline{C}$ be the large constant mentioned in that lemma. Set $x_* = Z^{\varepsilon-\frac{3}{5}}$. Then for $\overline{C} \le \ell \le Z^{10^{-9}}$, $V_\ell(r)$ satisfies the hypotheses of Theorem 1 in the section on Eigenvalue Sums for Degenerate Potentials.*

Proof. Hypotheses $(\overline{\text{Z0}})\dots(\overline{\text{Z8}})$ hold for $V_\ell(r)$, by virtue of Lemma 3 in the section on Approximate TF Potentials.(For those hypotheses, see section A.IVα.) Also, our I contains $\{V_\ell < 0\} = (x_{\rm left}(\ell), x_{\rm rt}(\ell))$, and $\ell \le Z^{1/5}$, so (CS1)...(CS6) hold as well.

The only remaining hypotheses in Theorem 1 on Eigenvalue Sums for Degenerate Potentials are the following.

$$\text{(18)} \qquad E_{\rm crit} < -\frac{3Z}{x_*}$$

$$V_\ell(x) > -\frac{4}{3}\frac{Z}{x_*} \quad \text{for } x > x_* \; . \tag{19}$$

We are using $E_{\text{crit}} = -Z^{18/10}$, $x_* = Z^{\varepsilon - 3/5}$, so (18) is obvious. Since $V_\ell(x) > V(x) > -(1+c_0)\frac{Z}{x}$ for all $x > 0$, (19) is also obvious. The proof of the Lemma. is complete. ■

¿From Lemma 3 above, and from Theorem 1 on Eigenvalue Sums for Degenerate Potentials, we conclude that

$$\text{sneg}(H_\ell) - \text{sneg}(H_\ell^c) = -\frac{2}{3\pi}\int_0^\infty \{\big(-V_\ell(r)\big)_+^{3/2} - \big(-V_\ell^c(r)\big)_+^{3/2}\}dr + \text{ Err}_\ell \tag{20}$$

$$\text{for } \overline{C} \le \ell \le Z^{10^{-9}} \;, \text{ with}$$

$$|\text{Err}_\ell| \le C\frac{Z}{x_*} = CZ^{\frac{8}{5}-\varepsilon} \; . \tag{21}$$

Next, suppose $Z^{10^{-9}} < \ell \le Z^{+1/5}$. Set $x_* = Z^{\varepsilon - 3/5}$, and take I, K as in Lemma 4 from the section on Approximate TF Potentials. That lemma shows that (Z0)...(Z9) hold for $V_\ell(r)$, $S(r) = \min\{\frac{Z}{r}, r^{-4}\}$, $B(r) = r$, with $\Lambda \sim \ell$. Also $\{V_\ell < 0\} \subset I$ by (Z0)...(Z9), and $\ell \le Z^{+1/5}$; hence, (CS1)...(CS6) hold for $V_\ell(r)$. Thus, the hypotheses of the Second WKB Eigenvalue Sum Theorem are satisfied. Applying that Theorem, we see that

$$\begin{aligned}\text{sneg}(H_\ell) - \text{sneg}(H_\ell^c) = \\ &-\frac{2}{3\pi}\int_0^\infty \{\big(-V_\ell(x)\big)_+^{3/2} - \big(-V_\ell^c(x)\big)_+^{3/2}\}dr \\ &+\frac{1}{24\pi}\int_0^\infty \{V_\ell''(x)\cdot\big(-V_\ell(x)\big)_+^{-1/2} - V_\ell^{c''}(x)\big(-V_\ell^c(x)\big)_+^{-1/2}\}dx \\ &+ \frac{\pi}{n_\ell}\tilde{\chi}(\phi_\ell) - \frac{2E_0^{3/2}}{Z}\tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}} - \sqrt{\ell(\ell+1)} - 1/2\Big) + \text{ Err}_\ell\end{aligned} \tag{22}$$

for $Z^{10^{-9}} < \ell \le Z^{+1/5}$ with

$$|\text{Err}_\ell| \le \Lambda^{5\varepsilon-2}\frac{Z}{x_*} \le \ell^{5\varepsilon-2}Z^{8/5} \; . \tag{23}$$

(See the definitions (6), (7) to check that (22) agrees with the conclusion of the Eigenvalue Sum Theorem.)

Next, suppose $Z^{1/5} \le \ell \le (1-\bar{c})\Omega$. Then Lemma 4 in the section on Approximate TF Potentials shows that $V_\ell(r)$ satisfies (Z0)...(Z9) with $\Lambda \sim \ell$. Therefore, the hypotheses of the First WKB Eigenvalue Sum Theorem are satisfied. Applying that theorem, we see that

$$\text{(24)} \quad \operatorname{sneg}(H_\ell) = -\frac{2}{3\pi}\int_0^\infty \big(-V_\ell(x)\big)_+^{3/2} dx + \frac{1}{24\pi}\int_0^\infty V_\ell''(x)\cdot\big(-V_\ell(x)\big)_+^{-1/2} dx + \frac{\pi}{n_\ell}\tilde{\chi}(\phi_\ell) + \text{Err}_\ell$$

for $Z^{+1/5} \le \ell \le (1-\bar{c})\Omega$, with

$$\text{(25)} \qquad |\text{Err}_\ell| \le \Lambda^{5\varepsilon-2}|\min_{r>0} V_\ell(r)| \sim C\ell^{5\varepsilon-2}\cdot\Big(\frac{Z^2}{\ell^2}\Big) \ .$$

To see that $\min_{r>0} V_\ell(r) \sim -\frac{Z^2}{\ell^2}$, we refer to equations (3)...(7) and (12), (13) in the section on Approximate TF Potentials.

Next, suppose $(1-\bar{c})\Omega \le \ell \le \Omega - \Omega^{1-10\varepsilon}$. Then Lemma 5 in the section on Approximate TF Potentials shows that (Z0)...(Z9) hold for $V_\ell(r)$, with $\tilde{S} = \frac{\Omega(\Omega-\ell)}{\check{r}^2}$, $\tilde{B}$ and I picked suitably, and $\Lambda \sim \Omega - \ell$. Hence $V_\ell(r)$, $\tilde{S}$, $\tilde{B}$, I satisfy the hypotheses of the First WKB Eigenvalue Sum Theorem. Applying that Theorem, we see that

$$\text{(26)} \quad \operatorname{sneg}(H_\ell) = -\frac{2}{3\pi}\int_0^\infty \big(-V_\ell(x)\big)_+^{3/2} dx + \frac{1}{24\pi}\int_0^\infty V_\ell''(x)\cdot\big(-V_\ell(x)\big)_+^{-1/2} dx + \frac{\pi}{n_\ell}\tilde{\chi}(\phi_\ell) + \text{Err}_\ell$$

for $(1-\bar{c})\Omega \le \ell \le \Omega - \Omega^{1-10\varepsilon}$, with

$$|\text{Err}_\ell| \le \Lambda^{5\varepsilon-2}|\min V_\ell(r)| \sim (\Omega-\ell)^{5\varepsilon-2}\tilde{S} = \frac{\Omega}{\check{r}^2}(\Omega-\ell)^{5\varepsilon-1} \ ,$$

i.e.

$$\text{(27)} \qquad |\text{Err}_\ell| \le Z(\Omega-\ell)^{5\varepsilon-1} \ .$$

Next we recall from the section on Approximate TF Potentials the following estimates. (See (14), (15) in that section.) For $(1-\bar{c})\Omega \le \ell < \Omega$, there are an $x_0(\ell) \sim Z^{-1/3}$ and an interval $I = \{|x - x_0(\ell)| < c_2 x_0(\ell)\}$ which satisfy:

$$\left|\left(\frac{d}{dx}\right)^\alpha V_\ell(x)\right| \le C_\alpha Z^{4/3}\big(x_0(\ell)\big)^{-\alpha} \quad \text{in } I \tag{28}$$

$$V_\ell''(x) \ge cZ^{4/3}\big(x_0(\ell)\big)^{-2} \quad \text{in } I \tag{29}$$

$$V_\ell'\big(x_0(\ell)\big) = 0 \ , -V_\ell\big(x_0(\ell)\big) \sim \frac{\Omega}{(x_0(\ell))^2}(\Omega - \ell) \sim Z(\Omega - \ell) \tag{30}$$

$$V_\ell(x) > \frac{c\ell^2}{x^2} \quad \text{outside } I \ . \tag{31}$$

Here $0 < c_2 < 1$ is a universal constant.

We use these observations to compute $\text{sneg}(H_\ell)$ for $\Omega - \Omega^{1-10\varepsilon} \le \ell < \Omega$.

Lemma 4. *Suppose $\Omega - \Omega^{1-10\varepsilon} \le \ell < \Omega$, and let ε, K, N be given. Assume Z is large enough, depending on ε, K, N and on the constants in (1) and (3). Pick $x_0 = x_0(\ell)$, $S = Z^{4/3}$, $B = x_0(\ell)$, I as in (28)...(31), $E_\infty = 0$. Then $V_\ell(r)$ satisfies the hypotheses (H0*)...(H6*) of the Third WKB Eigenvalue Sum Theorem. Moreover, $\lambda \sim Z^{1/3}$ and $-\lambda^{-3\varepsilon}S < V_\ell(x_0) < 0$.*

Proof. (H0*) just says that $0 < c_2 < 1$ in the definition of I. (H1*) is (28), (H2*) is (29), (H3*) is the first assertion of (30).

To prove (H4*) and (H5*), suppose $x \in (0,\infty)\backslash I$. Then $0 < x \le C|x - x_0|$, so (31) implies that $V_\ell(x) > \frac{c\ell^2}{x^2} > \frac{c'\ell^2}{|x-x_0|^2} > \frac{1000}{|x-x_0|^2}$ since $\ell \ge \Omega - \Omega^{1-10\varepsilon} \sim Z^{1/3}$. This implies (H5*) at once, and (H4*) also, since $\min\{E_\infty, V(x_0) + c''\lambda^{-2\varepsilon}S\} \le E_\infty = 0$.

(H6*) follows from the fact that we take Z large enough, since $\lambda = S^{1/2}B \sim (Z^{4/3})^{1/2}Z^{-1/3} = Z^{1/3}$. It remains to check that $-\lambda^{-3\varepsilon}S < V_\ell(x_0) < 0$. From (30) we get

$$0 < -V_\ell(x_0) < CZ(\Omega - \ell) \le CZ \cdot \Omega^{1-10\varepsilon} \sim Z^{\frac{4}{3} - \frac{10}{3}\varepsilon} \ .$$

On the other hand, $\lambda^{-3\varepsilon}S \sim (Z^{1/3})^{-3\varepsilon}Z^{4/3} \sim Z^{\frac{4}{3}-\varepsilon}$. Thus, $-\lambda^{-3\varepsilon}S < V_\ell(x_0) < 0$. The proof of Lemma 4 is complete. ■

Lemma 4 shows that $V_\ell(r)$ satisfies the hypotheses of the Third WKB Eigenvalue Sum Theorem when $\Omega - \Omega^{1-10\varepsilon} \le \ell < \Omega$. Applying that Theorem, we see that

$$(32)\quad \mathrm{sneg}(H_\ell) = -\frac{2}{3\pi}\int_0^\infty \big(-V_\ell(x)\big)_+^{3/2}dx + \frac{1}{24\pi}\int_0^\infty V_\ell''(x)\cdot\big(-V_\ell(x)\big)_+^{-1/2}dx + \frac{\pi}{n_\ell}\tilde{\chi}(\phi_\ell) + \mathrm{Err}_\ell$$

for $\Omega - \Omega^{1-10\varepsilon} \le \ell < \Omega$, with

$$(33)\qquad |\mathrm{Err}_\ell| \le \lambda^{5\varepsilon-2}S \sim (Z^{1/3})^{5\varepsilon-2}\cdot Z^{4/3} = Z^{\frac{2}{3}+\frac{5}{3}\varepsilon}\ .$$

We have succeeded in controlling $\mathrm{sneg}(H_\ell)$ for all ℓ ($0 \le \ell < \Omega$). Note that our results for $0 \le \ell \le Z^{1/5}$ compute $\mathrm{sneg}(H_\ell) - \mathrm{sneg}(H_\ell^c)$, while for $Z^{1/5} < \ell < \Omega$, we compute $\mathrm{sneg}(H_\ell)$.

Next, we will compute $\mathrm{sneg}(H_\ell^c)$ for $Z^{1/5} < \ell < \Omega_c$, which lets us compare $\mathrm{sneg}(H_\ell)$ with $\mathrm{sneg}(H_\ell^c)$ for all ℓ.

Take $0 < \bar{\bar{c}} << 1$. This constant will play a role analogous to $\bar{c}$ for the potentials V_ℓ^c.

Lemma 5. *Suppose $Z^{1/5} \le \ell \le (1-\bar{\bar{c}})\Omega_c$. Take $S(x) = \frac{Z}{x}$, $B(x) = x$, $I_{\mathrm{BVP}} = (0,\infty)$, $I = [10^{-9}\frac{\ell^2}{Z}, 10^9\frac{Z}{E_0}]$, $K = 10^{+9}$, $x_0 =$ critical point of $V_\ell^c = \frac{2\ell(\ell+1)}{Z}$, $\hat{c} =$ small constant. Then $V_\ell^c(r)$ satisfies the hypotheses (Z0)…(Z9) of the WKB Density Theorem, with $\Lambda \sim \ell$.*

Proof. This is a slight variant of a Lemma proven in the section on the Second WKB Eigenvalue Sum Theorem in [FS5]. We spell out the trivial details for the reader's convenience.

(Z0) says that $c < y/x < C$ and $c < (Zy^{-1})/(Zx^{-1}) < C$ for $|x-y| < cx$. That's obvious.

(Z1) says that $\left|\left(\frac{d}{dx}\right)^\alpha\left\{\frac{\ell(\ell+1)}{x^2}+E_0-\frac{Z}{x}\right\}\right| \le CZx^{-1-\alpha}$ in I.

We check the three terms $\frac{Z}{x}$, E_0, $\frac{\ell(\ell+1)}{x^2}$ separately. For $\frac{Z}{x}$, the desired estimate is obvious. For E_0, it's enough to take $\alpha=0$ and note that $|E_0| < 10^9\frac{Z}{x}$ in I. For $\frac{\ell(\ell+1)}{x^2}$, we write $\left|\left(\frac{d}{dx}\right)^\alpha\left\{\frac{\ell(\ell+1)}{x^2}\right\}\right| = c_\alpha \ell(\ell+1)x^{-2-\alpha} = c_\alpha\left\{\frac{\ell(\ell+1)}{Z}x^{-1}\right\}Zx^{-1-\alpha} \le C_\alpha Z^{-1-\alpha}$ in I. This proves (Z1).

(Z2) and (Z5) together say that $\{V_\ell^c<0\} = (x_{\rm left}, x_{\rm rt}) \subset I$ with dist $(x_{\rm left}, \partial I) > cx_{\rm left}$ and $\mathrm{dist}(x_{\rm rt},\partial I) > cx_{\rm rt}$. In fact, $\{V_\ell^c < 0\} = \{x^2V_\ell^c(x) < 0\} = \{\ell(\ell+1) - Zx + E_0x^2 < 0\}$, which has the form $(x_{\rm left}, x_{\rm rt})$ provided the discriminant $Z^2-4E_0\ell(\ell+1) > 0$. Now $\ell < (1-\bar{\bar{c}})\Omega_c$ with $\Omega_c(\Omega_c+1) = \max\limits_{x>0}\left(-x^2(E_0-\frac{Z}{x})\right) = \max\limits_{x>0}\left(Zx-E_0x^2\right) = \frac{Z^2}{4E_0}$. Hence $\ell(\ell+1) < (1-\bar{\bar{c}})\Omega_c(\Omega_c+1) = (1-\bar{\bar{c}})\frac{Z^2}{4E_0}$, so that $Z^2-4E_0\ell(\ell+1) > \bar{\bar{c}}Z^2 > 0$, as needed.

Note that $x_{\rm left} = \frac{Z-\sqrt{Z^2-4E_0\ell(\ell+1)}}{2E_0}$, $x_{\rm rt} = \frac{Z+\sqrt{Z^2-4E_0\ell(\ell+1)}}{2E_0}$, so that $x_{\rm left} > 0$ and $x_{\rm rt} < \frac{2Z}{2E_0}$. Hence $\{V_\ell^c < 0\} = (x_{\rm left}, x_{\rm rt}) \subset (0, \frac{Z}{E_0})$. For $0 < x < \frac{\ell(\ell+1)}{Z}$ we have $V_\ell^c > \frac{\ell(\ell+1)}{x^2} - \frac{Z}{x} > 0$, so

$$\text{(33bis)} \qquad \{V_\ell^c < 0\} = (x_{\rm left}, x_{\rm rt}) \subset \left[\frac{\ell(\ell+1)}{Z}, \frac{Z}{E_0}\right] .$$

This implies $(x_{\rm left}, x_{\rm rt}) \subset I$ and $\mathrm{dist}(x_{\rm left},\partial I) > cx_{\rm left}$ and $\mathrm{dist}(x_{\rm rt},\partial I) > cx_{\rm rt}$, by definition of I. This completes the proof of (Z2) and (Z5).

(Z3) is proven as follows. We have $x_0^2V_\ell^c(x_0) = \ell(\ell+1) - Zx_0 + E_0x_0^2 = \ell(\ell+1) - 2\ell(\ell+1) + E_0\cdot\frac{4\ell^2(\ell+1)^2}{Z^2} = -\ell(\ell+1)\left[1-\frac{4E_0}{Z^2}\ell(\ell+1)\right]$. Also $0<\ell\le(1-\bar{\bar{c}})\Omega_c$, so $\ell(\ell+1) \le (1-\bar{\bar{c}})\Omega_c(\Omega_c+1) = (1-\bar{\bar{c}})\max\limits_{x>0}\left(-x^2(E_0-\frac{Z}{x})\right)$ by definition of Ω_c. The max. of $-x^2(E_0-\frac{Z}{x}) = Zx-E_0x^2$ is $\frac{Z^2}{4E_0}$, attained at $x=\frac{Z}{2E_0}$, so that $\ell(\ell+1) \le (1-\bar{\bar{c}})\cdot\frac{Z^2}{4E_0}$. Therefore, $-x_0^2V_\ell^c(x_0) = \ell(\ell+1)\cdot\left[1-\frac{4E_0}{Z^2}\ell(\ell+1)\right] \ge \bar{\bar{c}}\ell(\ell+1)$, so $-V_\ell^c(x_0) \ge \bar{\bar{c}}\frac{\ell(\ell+1)}{x_0^2} \ge c'\frac{Z}{x_0}$ because $x_0 = 2\ell(\ell+1)Z^{-1}$. Thus $V_\ell^c(x_0) \le -c'S(x_0)$ for $S(x) = \frac{Z}{x}$. The derivatives of V_ℓ^c are given by

$$\text{(34)} \qquad (V_\ell^c)'(x) = -\frac{2\ell(\ell+1)}{x^3} + \frac{Z}{x^2} = \frac{Zx-2\ell(\ell+1)}{x^3} = \frac{Z}{x^2}\cdot\frac{[x-x_0]}{x}$$

and

$$(35) \qquad (V_\ell^c)'' = +\frac{6\ell(\ell+1)}{x^4} - \frac{2Z}{x^3} = \frac{6\ell(\ell+1) - 2Zx}{x^4} \ .$$

From (34), we have $(V_\ell^c)'(x_0) = 0$. If $|x - x_0| < c_1 x_0$, then $2Zx = 4\ell(\ell+1) + 2Z[x - x_0] = \{4 + O(c_1)\}\ell(\ell+1)$. Hence if c_1 is small and $|x - x_0| < c_1 x_0$, then (35) shows that $(V_\ell^c)'' \geq \frac{(\text{const.})\ell(\ell+1)}{x^4} \geq (\text{const.}) \frac{\ell(\ell+1)}{x_0^4} \sim \frac{Z}{x_0^3}$ since $x \sim x_0 \sim \ell(\ell+1)Z^{-1}$. Thus, $V_\ell^c(x_0) < -cS(x_0)$, $(V_\ell^c)'(x_0) = 0$, and $(V_\ell^c)''(x) > cS(x_0)B^{-2}(x_0)$ for $|x - x_0| < c_1 B(x_0)$. These are the assertions of (Z3).

(Z4) is proven as follows.

Suppose $x_{\text{left}} \leq x \leq x_0 - c_1 x_0$. From (34) we get $-(V_\ell^c)'(x) \geq c_1 \frac{Z}{x^2} = c_1 S(x) B^{-1}(x)$, since $\frac{x_0 - x}{x} \geq \frac{c_1 x_0}{x_0}$. This is the first assertion of (Z4).

On the other hand, suppose $x_0 + c_1 x_0 \leq x \leq x_{\text{rt}}$. Then (34) implies $+(V_\ell^c)'(x) \geq c\frac{Z}{x^2} = cS(x)B^{-1}(x)$, since $\frac{x - x_0}{x} > 1 - \frac{1}{1+c_1} = c > 0$. This is the remaining assertion of (Z4).

(Z5) has already been proven, together with (Z2). Let us compute $\Lambda = \left(\int_{x_{\text{left}}}^{x_{\text{rt}}} \frac{dx}{S^{1/2}(x)x^2}\right)^{-1}$. Since $|(V_\ell^c)'(x)| \leq \frac{CZ}{x^2}$ in $[x_{\text{left}}, x_0]$ by (Z1), while $V_\ell^c(x_{\text{left}}) = 0$ by definition, and $(V_\ell^c)(x_0) < -\frac{cZ}{x_0}$ by (Z3), it follows that $x_{\text{left}} \leq (1 - c)x_0$ for a small, positive constant c. Hence $x_{\text{rt}}/x_{\text{left}} > x_0/x_{\text{left}} > 1 + c'$ for a small, positive constant c'. So $\Lambda^{-1} = \int_{x_{\text{left}}}^{x_{\text{rt}}} \frac{dx}{(\frac{Z}{x})^{1/2}x^2} = Z^{-1/2}\int_{x_{\text{left}}}^{x_{\text{rt}}} \frac{dx}{x^{3/2}} \sim Z^{-1/2}x_{\text{left}}^{-1/2}$. From (33 bis) and $x_{\text{left}} < x_0 = 2\ell(\ell+1)Z^{-1}$, we conclude that $x_{\text{left}} \sim \ell(\ell+1)Z^{-1} \sim \ell^2 Z^{-1}$ since we take $\ell \geq Z^{1/5} >> 1$. Hence $\Lambda^{-1} \sim Z^{-1/2}(\ell^2 Z^{-1})^{-1/2} = \ell^{-1}$, so $\Lambda \sim \ell$ as claimed in the statement of Lemma 5.

(Z6) is proven as follows. The assertion of (Z6) about $x \in I_{\text{BVP}}$ with $x < x_{\text{left}} - \Lambda^K B(x_{\text{left}})$ holds vacuously, since $I_{\text{BVP}} = (0, \infty)$ and $x_{\text{left}} - \Lambda^K B(x_{\text{left}}) = x_{\text{left}} \cdot (1 - \Lambda^K)$ is negative. For $x > x_{\text{rt}} + \Lambda^K B(x_{\text{rt}})$, we must show that $V_\ell^c(x) \geq \frac{1000}{|x - x_{\text{rt}}|^2}$.

By the formula $x_{\text{rt}} = \frac{Z + \sqrt{Z^2 - 4E_0\ell(\ell+1)}}{2E_0}$, we have $x_{\text{rt}} \sim \frac{Z}{E_0}$. If $x > 10^9 \frac{Z}{E_0}$, then $V_\ell^c(x) \geq E_0 - \frac{Z}{x} > \frac{1}{2}E_0 > 1000$ since $E_0 \sim Z^{4/3}$. For $x > x_{\text{rt}} + \Lambda^K x_{\text{rt}}$ we have $x - x_{\rm rt} > (c\ell)^K\left(\frac{cZ}{E_0}\right) \geq (cZ^{1/5})^K \cdot cZ^{-1/3} > Z$ since $K = 10^{+9}$. Hence for $x > x_{\rm rt} + \Lambda^K x_{\rm rt}$, we have $V^c_\ell(x) > 1000 > \frac{1000}{(x-x_{\rm rt})^2}$, which is the assertion of (Z6).

(Z7) amounts to saying that $(x_{\rm rt}/x_{\rm left}) \leq \Lambda^K$.

We saw that $x_{\rm left} \sim \ell(\ell+1)Z^{-1} > Z^{-1}$ for $\ell \geq Z^{\frac{1}{5}}$, and that $x_{\rm rt} \sim \frac{Z}{E_0} \sim Z^{-1/3}$. So (Z7) follows if we have $CZ^{2/3} \leq \Lambda^K$. Since $\Lambda \sim \ell \geq Z^{1/5}$ while $K = 10^{+9}$, this is obvious. So (Z7) holds.

(Z8) holds, simply because we pick $\hat{c}$ small enough, and

(Z9) holds because $\Lambda \sim \ell \geq Z^{1/5}$ and we take Z large enough. The proof of Lemma 5 is complete. ■

Lemma 5 and the first WKB Eigenvalue Sum Theorem show that

(36) $$\text{sneg}(H^c_\ell) = -\frac{2}{3\pi}\int_0^\infty \left(-V^c_\ell(x)\right)_+^{3/2} dx + \frac{1}{24\pi}\int_0^\infty (V^c_\ell)''(x)\cdot\left(-V^c_\ell(x)\right)_+^{-1/2} dx + \frac{\pi}{n^c_\ell}\tilde{\chi}(\phi^c_\ell) + \text{Err}^c_\ell \quad \text{for } Z^{1/5} \leq \ell \leq (1-\overline{\overline{c}})\Omega_c \text{ , with}$$

(37) $$n^c_\ell = \int_0^\infty \left(-V^c_\ell(x)\right)_+^{-1/2} dx$$

(38) $$\phi^c_\ell = \frac{1}{\pi}\int_0^\infty \left(-V^c_\ell(x)\right)_+^{1/2} dx - \frac{1}{2} \ ,$$

(39) $$|\text{Err}^c_\ell| \leq \Lambda^{5\varepsilon-2}|\min_{x>0} V^c_\ell(x)| \sim \ell^{5\varepsilon-2}\cdot\frac{Z^2}{\ell^2} \ .$$

In the discussion of elementary integrals in the Review of Earlier Results, we saw that

(40) $$\frac{\pi}{n^c_\ell}\tilde{\chi}(\phi^c_\ell) = \frac{2E_0^{3/2}}{Z}\tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}} - \sqrt{\ell(\ell+1)} - \frac{1}{2}\Big) \quad \text{for } 0 < \ell < \Omega_c \ .$$

Substituting this into (36), we obtain

(41) $$\text{sneg}(H^c_\ell) = -\frac{2}{3\pi}\int_0^\infty \left(-V^c_\ell(x)\right)_+^{3/2} dx + \frac{1}{24\pi}\int_0^\infty V^{c''}_\ell(x)\left(-V^c_\ell(x)\right)_+^{-1/2} dx + \frac{2E_0^{3/2}}{Z}\tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}} - \sqrt{\ell(\ell+1)} - \frac{1}{2}\Big) + \text{Err}^c_\ell \quad \text{for } Z^{1/5} < \ell \leq (1-\overline{\overline{c}})\Omega_c, \text{ with}$$

$$|\mathrm{Err}_\ell^c| \le C\ell^{5\varepsilon-4}Z^2 \ . \tag{42}$$

To compute $\mathrm{sneg}(H_\ell^c)$ for $(1-\bar{\bar{c}})\Omega_c \le \ell < \Omega_c$, we use the following elementary observation.

Lemma 6. *Suppose* $(1-\bar{\bar{c}})\Omega_c \le \ell < \Omega_c$*; and set* $x_0 = 2\ell(\ell+1)Z^{-1}$*, and* $I = \{|x-x_0| < \frac{1}{10}x_0\}$*. Then*

$$\left|\left(\frac{d}{dx}\right)^\alpha V_\ell^c(x)\right| \le C_\alpha Z^{4/3}x_0^{-\alpha} \quad \textit{in } I \tag{43}$$

$$\left(\frac{d}{dx}\right)^2 V_\ell^c(x) \ge cZ^{4/3}x_0^{-2} \quad \textit{in } I \tag{44}$$

$$\left(\frac{d}{dx}V_\ell^c\right)(x_0) = 0 \quad \textit{and} \quad -V_\ell^c(x_0) \sim \frac{\Omega_c}{x_0^2}(\Omega_c-\ell) \sim Z(\Omega_c-\ell) \tag{45}$$

$$V_\ell^c(x) \ge \frac{c\ell^2}{x^2} \quad \textit{outside } I \ . \tag{46}$$

Proof. Note that $\ell \sim Z^{1/3}$, $\Omega_c \sim Z^{1/3}$, $x_0 \sim Z^{-1/3}$. We have

$$\begin{aligned}\left(\frac{d}{dx}\right)^\alpha\left\{\frac{\ell(\ell+1)}{x^2}\right\} &= c_\alpha\frac{\ell(\ell+1)}{x^{2+\alpha}} \sim Z^{4/3}x_0^{-\alpha} \text{ in } I \ ,\\ \left(\frac{d}{dx}\right)^\alpha\{E_0\} &\sim Z^{4/3}x_0^{-\alpha} \text{ if } \alpha=0 \ , \ 0 \text{ otherwise}\\ \left(\frac{d}{dx}\right)^\alpha\left\{\frac{Z}{x}\right\} &= c'_\alpha\frac{Z}{x^{1+\alpha}} \sim Z^{4/3}x_0^{-\alpha} \text{ in } I \ .\end{aligned}$$

This proves (43). To prove (44), recall that $(V_\ell^c)''(x) = \frac{6\ell(\ell+1)-2Zx}{x^4} \ge \frac{6\ell(\ell+1)-2Z\cdot\frac{11}{10}\cdot 2\ell(\ell+1)Z^{-1}}{x^4}$ for $x \in I$. Thus $x \in I$ implies $(V_\ell^c)''(x) \ge \frac{\ell(\ell+1)}{x^4} \sim \frac{\ell(\ell+1)}{x_0^2}\cdot\frac{1}{x_0^2} \sim Z^{4/3}x_0^{-2}$, proving (44).

Next, we check (45). We have

$$(V_\ell^c)'(x_0) = -\frac{2\ell(\ell+1)}{x_0^3} + \frac{Z}{x_0^2} = 0 \ , \text{ and} \tag{47}$$

(48)
$$-x_0^2V_\ell^c(x_0) = -\ell(\ell+1) + Zx_0 - E_0x_0^2 = -\ell(\ell+1) + 2\ell(\ell+1) - E_0 \cdot \frac{4\ell^2(\ell+1)^2}{Z^2}$$
$$= \ell(\ell+1)\big[1 - \frac{4E_0}{Z^2}\ell(\ell+1)\big] \ .$$

Since $\Omega_c(\Omega_c+1) = \max_{x>0}\big(-x^2(E_0 - \frac{Z}{x})\big) = \frac{Z^2}{4E_0}$, (48) may be rewritten as

$$-x_0^2V_\ell^c(x_0) = \ell(\ell+1)\big[1 - \frac{\ell(\ell+1)}{\Omega_c(\Omega_c+1)}\big] = \frac{\ell(\ell+1)}{\Omega_c(\Omega_c+1)}[\Omega_c(\Omega_c+1) - \ell(\ell+1)]$$
$$\sim [\Omega_c(\Omega_c+1) - \ell(\ell+1)] \sim \Omega_c(\Omega_c - \ell) \text{ for } (1-\overline{\overline{c}})\Omega_c \le \ell < \Omega_c \ .$$

Thus $-V_\ell^c(x_0) \sim \frac{\Omega_c}{x_0^2}(\Omega_c - \ell) \sim Z(\Omega_c - \ell)$. This and (47) prove (45). It remains to check (46). We argue as follows.

$$x^2V_\ell^c(x) = [\Omega_c(\Omega_c+1) + E_0x^2 - Zx] + [\ell(\ell+1) - \Omega_c(\Omega_c+1)]$$
$$= [\frac{Z^2}{4E_0} + E_0x^2 - Zx] - [\Omega_c(\Omega_c+1) - \ell(\ell+1)]$$
$$= E_0(x - \frac{Z}{2E_0})^2 - [\Omega_c(\Omega_c+1) - \ell(\ell+1)]$$
$$= E_0(x - 2(\Omega_c)(\Omega_c+1)Z^{-1})^2 - [\Omega_c(\Omega_c+1) - \ell(\ell+1)] \ . \tag{49}$$

For $x \notin I$ and $(1-\overline{\overline{c}})\Omega_c \le \ell < \Omega_c$, we have

$$|x - 2\Omega_c(\Omega_c+1)Z^{-1}| \ge |x - 2\ell(\ell+1)Z^{-1}| - 2Z^{-1}|\Omega_c(\Omega_c+1) - \ell(\ell+1)|$$
$$\ge \frac{1}{10}\cdot 2\ell(\ell+1)Z^{-1} - 6Z^{-1}\Omega_c(\Omega_c - \ell)$$
$$\ge \frac{1}{10}\Omega_c(\Omega_c+1)Z^{-1} - 6\overline{\overline{c}}Z^{-1}\Omega_c^2$$
$$\ge \frac{1}{20}Z^{-1}\Omega_c^2 \quad \text{since } \overline{\overline{c}} \text{ is small} \ . \tag{50}$$

Also for $(1-\overline{\overline{c}})\Omega_c \le \ell < \Omega_c$ we have

$$[\Omega_c(\Omega_c+1) - \ell(\ell+1)] \le 3\Omega_c(\Omega_c - \ell) \le 3\overline{\overline{c}}\,\Omega_c^2 \ . \tag{51}$$

Putting (50) and (51) into (49), we see that

$$x^2V_\ell^c(x) \ge E_0 \cdot (\frac{1}{20}Z^{-1}\Omega_c^2)^2 - 3\overline{\overline{c}}\,\Omega_c^2 \ .$$

The first term on the right-hand side is $\sim Z^{4/3}\cdot(Z^{-1}Z^{2/3})^2\sim Z^{2/3}$, while the second term is $\sim \bar{\bar{c}}Z^{2/3}$.

Since $\bar{\bar{c}}$ is taken small, we have

$$x^2V_\ell^c(x)\geq cZ^{2/3}\sim\ell^2\quad\text{for } x\notin I \text{ and } (1-\bar{\bar{c}})\Omega_c\leq\ell<\Omega_c\ .$$

This is equivalent to (46). The proof of Lemma 6 is complete. ■

Our first application of Lemma 6 is as follows.

Lemma 7. *Suppose* $(1-\bar{\bar{c}})\Omega_c\leq\ell<\Omega_c-c\Omega_c^{7/43}$. *Set* $x_0=2\ell(\ell+1)Z^{-1}$, *take* $\tilde{S}=\frac{\Omega_c(\Omega_c-\ell)}{\check{r}_c^2}$, $\tilde{B}=\frac{\check{r}_c(\Omega_c-\ell)^{1/2}}{\Omega_c^{1/2}}$, *and define* $I=[x_0-h,x_0+h]$, *with* $h=\min\left(\frac{1}{10}x_0,\underline{C}\tilde{B}\right)$ *for a large constant* $\underline{C}$. *Let* ε, N *be given. Set* $K=100^{90}$, *and let* $\hat{c}$ *be a small enough constant. Then the potential* $V_\ell^c(r)$, *the weights* $\tilde{S}$, $\tilde{B}$ *and the interval* I *satisfy the hypotheses (Z0)…(Z9) of the First WKB Eigenvalue Sum Theorem, with* $\Lambda\sim(\Omega_c-\ell)$.

Sketch of Proof. Repeat the proof of Lemma 5 in the section on the Density in an Approximate TF Potential in [FS7], replacing equations (14) and (15) in that section by Lemma 6 above. ■

¿From Lemma 7 and the First WKB Eigenvalue Sum Theorem, we see that

$$\operatorname{sneg}(H_\ell^c)=-\frac{2}{3\pi}\int_0^\infty\left(-V_\ell^c(x)\right)_+^{3/2}dx+\frac{1}{24\pi}\int_0^\infty(V_\ell^c)''(x)\cdot\left(-V_\ell^c(x)\right)_+^{-1/2}dx$$
$$+\frac{\pi}{n_\ell^c}\tilde{\chi}(\phi_\ell^c)+\ \mathrm{Err}_\ell^c$$

for $(1-\bar{\bar{c}})\Omega_c\leq\ell\leq\Omega_c-\Omega_c^{1-10\,\varepsilon}$, with

$$|\mathrm{Err}_\ell^c|\leq\Lambda^{5\varepsilon-2}\cdot|\min_{x>0}V_\ell^c(x)|\sim(\Omega_c-\ell)^{5\varepsilon-2}\tilde{S}=\frac{\Omega_c}{\check{r}_c^2}(\Omega_c-\ell)^{5\varepsilon-1}\ ,$$

i.e. $|\mathrm{Err}_\ell^c|\leq CZ(\Omega_c-\ell)^{5\varepsilon-1}$.

Recalling the formula (40) for $\frac{\pi}{n_\ell^c}\tilde{\chi}(\phi_\ell^c)$, we obtain

$$\text{(52)}\quad \operatorname{sneg}(H_\ell^c) = -\frac{2}{3\pi}\int_0^\infty \big(-V_\ell^c(x)\big)_+^{3/2} dx + \frac{1}{24\pi}\int_0^\infty (V_\ell^c)''(x)\cdot\big(-V_\ell^c(x)\big)_+^{-1/2} dx + \frac{2E_0^{3/2}}{Z}\tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}} - \sqrt{\ell(\ell+1)} - \frac{1}{2}\Big) + \ \mathrm{Err}_\ell^c$$

for $(1-\overline{\overline{c}})\Omega_c \le \ell \le \Omega_c - \Omega_c^{1-10\,\varepsilon}$, with

$$\text{(53)}\qquad |\mathrm{Err}_\ell^c| \le CZ(\Omega_c - \ell)^{5\varepsilon - 1}\ .$$

The second application of Lemma 6 is as follows.

Lemma 8. *Suppose* $\Omega_c - \Omega_c^{1-10\varepsilon} \le \ell < \Omega_c$, *and let* ε, K, N *be given. Suppose* Z *is large enough, depending on* ε, K, N *and the constants in (1), (3). Pick* $x_0 = 2\ell(\ell+1)Z^{-1}$, $S = Z^{4/3}$, $B = x_0$, $I = \{|x - x_0| < \frac{1}{10}x_0\}$. *Then* $V_\ell^c(r)$ *satisfies the hypotheses (H0*)... (H6*) of the Third WKB Eigenvalue Sum Theorem. Moreover,* $\lambda \sim Z^{+1/3}$ *and* $-\lambda^{-3\varepsilon}S < V_\ell^c(x_0) < 0$.

Sketch of Proof. Just repeat the proof of Lemma 4, using Lemma 6 in place of (28)...(31).

Lemma 8 shows that $V_\ell^c(r)$ satisfies the hypotheses of the Third WKB Eigenvalue Sum Theorem, when $\Omega_c - \Omega_c^{1-10\varepsilon} \le \ell < \Omega_c$. Applying that Theorem, we see that

$$\operatorname{sneg}(H_\ell^c) = -\frac{2}{3\pi}\int_0^\infty \big(-V_\ell^c(x)\big)_+^{3/2} dx + \frac{1}{24\pi}\int_0^\infty V_\ell^{c''}(x)\big(-V_\ell^c(x)\big)_+^{-1/2} dx + \frac{\pi}{n_\ell^c}\tilde{\chi}(\phi_\ell^c) + \ \mathrm{Err}_\ell^c$$

for $\Omega_c - \Omega_c^{1-10\varepsilon} \le \ell < \Omega_c$, with

$$|\mathrm{Err}_\ell^c| \le \lambda^{5\varepsilon-2}S \sim (Z^{1/3})^{5\varepsilon-2}(Z^{4/3}) = Z^{\frac{2}{3}+\frac{5}{3}\varepsilon}\ .$$

Using (40) to evaluate $\frac{\pi}{n_\ell^c}\tilde{\chi}(\phi_\ell^c)$, we obtain

$$\text{(54)}\quad \operatorname{sneg}(H_\ell^c) = -\frac{2}{3\pi}\int_0^\infty \big(-V_\ell^c(x)\big)_+^{3/2} dx + \frac{1}{24\pi}\int_0^\infty V_\ell^{c''}(x)\big(-V_\ell^c(x)\big)_+^{-1/2} dx + \frac{2E_0^{3/2}}{Z}\tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}} - \sqrt{\ell(\ell+1)} - \frac{1}{2}\Big) + \ \mathrm{Err}_\ell^c$$

for $\Omega_c - \Omega_c^{1-10\varepsilon} \le \ell < \Omega_c$, with

$$|\mathrm{Err}_\ell^c| \le C Z^{\frac{2}{3}+\frac{5}{3}\varepsilon} \; . \tag{55}$$

We have enough information to control $\mathrm{sneg}(H_\ell) - \mathrm{sneg}(H_\ell^c)$ for all ℓ. We will use what we have learned to compute $\mathrm{sneg}(H) - \mathrm{sneg}(H_c)$, where

$$H = -\Delta + V(|x|) \quad \text{and} \quad H_c = -\Delta + E_0 - \frac{Z}{|x|} \quad \text{on} \quad \mathbb{R}^3 \; .$$

Recall that $\mathrm{sneg}(H) = \sum_{0 \le \ell < \Omega} (2\ell+1)\mathrm{sneg}(H_\ell)$, $\mathrm{sneg}(H_c) = \sum_{0 \le \ell < \Omega_c} (2\ell+1)\mathrm{sneg}(H_\ell^c)$. Hence,

$$\begin{aligned} \mathrm{sneg}(H) - \; \mathrm{sneg}(H_c) = & \\ \sum_{0 \le \ell \le Z^{1/5}} (2\ell+1)\big[\mathrm{sneg}(H_\ell) - \mathrm{sneg}(H_\ell^c)\big] &+ \sum_{Z^{1/5} < \ell < \Omega} (2\ell+1)\mathrm{sneg}(H_\ell) \\ &- \sum_{Z^{1/5} < \ell < \Omega_c} (2\ell+1)\mathrm{sneg}(H_\ell^c) \; . \end{aligned} \tag{56}$$

Let $\overline{C}$ be the large constant in (20). We use (20), (21) for $\overline{C} \le \ell \le Z^{10^{-9}}$; we use (16), (17) for $1 \le \ell < \overline{C}$; and we use (11), (12) for $\ell = 0$. Thus, we have

$$\mathrm{sneg}(H_\ell) - \mathrm{sneg}(H_\ell^c) = -\frac{2}{3\pi} \int_0^\infty \big\{\big(-V_\ell(x)\big)_+^{3/2} - \big(-V_\ell^c(x)\big)_+^{3/2}\big\} dx + \; \mathrm{Error}_\ell$$

for $0 \le \ell \le Z^{10^{-9}}$, with $|\mathrm{Error}_\ell| \le Z^{8/5}$. Therefore,

$$\begin{aligned} &\sum_{0 \le \ell \le Z^{10^{-9}}} (2\ell+1)[\mathrm{sneg}(H_\ell) - \mathrm{sneg}(H_\ell^c)] \\ &= -\frac{2}{3\pi} \sum_{0 \le \ell \le Z^{10^{-9}}} (2\ell+1) \int_0^\infty \big\{\big(-V_\ell(x)\big)_+^{3/2} - \big(-V_\ell^c(x)\big)_+^{3/2}\big\} dx + \; \mathrm{Error}^A \; , \end{aligned} \tag{57}$$

with

$$|\mathrm{Error}^A| \le C \, Z^{\frac{8}{5}+2\cdot 10^{-9}} \; . \tag{58}$$

We combine (57), (58) with (22), (23). Since

$$\sum_{Z^{10^{-9}} < \ell \le Z^{1/5}} (2\ell+1)|\mathrm{Err}_\ell| \le \sum_{Z^{10^{-9}} < \ell \le Z^{1/5}} C\ell^{5\varepsilon-1} Z^{8/5} \le C' Z^{\frac{8}{5}+\varepsilon} \; ,$$

the result is as follows.

$$(59)\qquad \sum_{0\le\ell\le Z^{1/5}} (2\ell+1)\big[\mathrm{sneg}(H_\ell)-\mathrm{sneg}(H_\ell^c)\big]$$

$$= -\frac{2}{3\pi}\sum_{0\le\ell\le Z^{1/5}}(2\ell+1)\int_0^\infty \big\{\big(-V_\ell(x)\big)_+^{3/2}-\big(-V_\ell^c(x)\big)_+^{3/2}\big\}dx$$

$$+\frac{1}{24\pi}\sum_{Z^{10^{-9}}<\ell\le Z^{1/5}}(2\ell+1)\int_0^\infty\big\{V_\ell''(x)\cdot\big(-V_\ell(x)\big)_+^{-1/2}-V_\ell^{c''}(x)\cdot\big(-V_\ell^c(x)\big)_+^{-1/2}\big\}dx$$

$$+\sum_{Z^{10^{-9}}<\ell\le Z^{1/5}}(2\ell+1)\frac{\pi}{n_\ell}\tilde\chi(\phi_\ell)$$

$$-\sum_{Z^{10^{-9}}<\ell\le Z^{1/5}}(2\ell+1)\cdot\frac{2E_0^{3/2}}{Z}\tilde\chi\Big(\frac{Z}{2E_0^{1/2}}-\sqrt{\ell(\ell+1)}-\frac12\Big)$$

$$+\ \mathrm{Error}^B\ ,\qquad \text{with}$$

$$(59\text{bis})\qquad |\mathrm{Error}^B|\le C\,Z^{\frac85+2\cdot10^{-9}}\ .$$

Thus, we have evaluated the first term on the right in (56).

Next, we evaluate the second term on the right. From (24), (26), (32), we get

$$(60)\qquad \sum_{Z^{1/5}<\ell<\Omega}(2\ell+1)\mathrm{sneg}(H_\ell)$$

$$= -\frac{2}{3\pi}\sum_{Z^{1/5}<\ell<\Omega}(2\ell+1)\int_0^\infty\big(-V_\ell(x)\big)_+^{3/2}dx+\frac{1}{24\pi}\sum_{Z^{1/5}<\ell<\Omega}(2\ell+1)\int_0^\infty V_\ell''(x)\cdot\big(-V_\ell(x)\big)_+^{-1/2}dx$$

$$+\sum_{Z^{1/5}<\ell<\Omega}(2\ell+1)\cdot\frac{\pi}{n_\ell}\tilde\chi(\phi_\ell)+\ \mathrm{Error}^C\ ,$$

with $\mathrm{Error}^C=\sum_{Z^{1/5}<\ell<\Omega}(2\ell+1)\ \mathrm{Err}_\ell$. By (25), (27), (33) we have

$$|\mathrm{Error}^C|\le\sum_{Z^{1/5}<\ell\le(1-\bar c)\Omega}(2\ell+1)\cdot CZ^2\ell^{5\varepsilon-4}+\sum_{(1-\bar c)\Omega<\ell\le\Omega-\Omega^{1-10\varepsilon}}(2\ell+1)\cdot Z(\Omega-\ell)^{5\varepsilon-1}$$

$$+\sum_{\Omega-\Omega^{1-10\varepsilon}<\ell<\Omega}(2\ell+1)\cdot Z^{\frac23+\frac53\varepsilon}\ .$$

Here, the first sum on the right is $\sim Z^2(Z^{\frac15})^{5\varepsilon-2}=Z^{\frac85+\varepsilon}$, the second sum on the right is $\sim\Omega\cdot Z\cdot\Omega^{5\varepsilon}\sim Z^{\frac43+\frac53\varepsilon}$, and the third sum is $\sim Z^{1+\frac53\varepsilon}\cdot\Omega^{1-10\varepsilon}\sim Z^{\frac43-\frac53\varepsilon}$.

Therefore,

$$|\mathrm{Error}^C| \le CZ^{\frac{8}{5}+\varepsilon} \; . \tag{61}$$

So we have evaluated the second term on the right in (56). To evaluate the last term in (56), we combine (41), (52), (54), obtaining

$$\begin{aligned}
\sum_{Z^{1/5}<\ell<\Omega_c} (2\ell+1)\mathrm{sneg}(H_\ell^c) \\
&= -\frac{2}{3\pi} \sum_{Z^{1/5}<\ell<\Omega_c} (2\ell+1)\cdot \int_0^\infty \big(-V_\ell^c(x)\big)_+^{3/2} dx \\
&+ \frac{1}{24\pi} \sum_{Z^{1/5}<\ell<\Omega_c} (2\ell+1) \int_0^\infty V_\ell^{c''}(x)\cdot \big(-V_\ell^c(x)\big)_+^{-1/2} dx \\
&+ \sum_{Z^{1/5}<\ell<\Omega_c} (2\ell+1)\cdot \frac{2E_0^{3/2}}{Z} \tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}} - \sqrt{\ell(\ell+1)} - \frac{1}{2}\Big) \\
&+ \mathrm{Error}^D \; ,
\end{aligned} \tag{62}$$

with $\mathrm{Error}^D = \sum_{Z^{1/5}<\ell<\Omega_c} (2\ell+1)\mathrm{Err}_\ell^c$.

By (42), (53), (55) we have

$$\begin{aligned}
|\mathrm{Error}^D| \le \sum_{Z^{1/5}<\ell<(1-\bar{\bar{c}})\Omega_c} (2\ell+1)\cdot C\ell^{5\varepsilon-4}Z^2 + \sum_{(1-\bar{\bar{c}})\Omega_c\le\ell<\Omega_c-\Omega_c^{1-10\varepsilon}} (2\ell+1)\cdot CZ\cdot(\Omega_c-\ell)^{5\varepsilon-1} \\
+ \sum_{\Omega_c-\Omega_c^{1-10\varepsilon}\le\ell<\Omega_c} (2\ell+1)\cdot CZ^{\frac{2}{3}+\frac{5}{3}\varepsilon} \; ,
\end{aligned}$$

and therefore

$$|\mathrm{Error}^D| \le CZ^{\frac{8}{5}+\varepsilon} \; , \qquad \text{as in (60), (61)} \; . \tag{63}$$

We have evaluated all the terms on the right in (56). Substituting (59), (60),

(62) into (56), we see that

$$\begin{aligned}
&\operatorname{sneg}(H)-\operatorname{sneg}(H_c)\\
&=-\frac{2}{3\pi}\sum_{\ell\geq 0}(2\ell+1)\int_0^\infty\{(-V_\ell(x))_+^{3/2}-(-V_\ell^c(x))_+^{3/2}\}dx\\
&+\frac{1}{24\pi}\sum_{\ell>Z^{10^{-9}}}(2\ell+1)\int_0^\infty\{V_\ell''(x)\cdot(-V_\ell(x))_+^{-1/2}-V_\ell^{c''}(x)\cdot(-V_\ell^c(x))_+^{-1/2}\}dx\\
&+\pi\sum_{\Omega>\ell>Z^{10^{-9}}}\frac{(2\ell+1)}{n_\ell}\tilde{\chi}(\phi_\ell)\\
&-\sum_{Z^{10^{-9}}<\ell<\Omega_c}(2\ell+1)\cdot\frac{2E_0^{3/2}}{Z}\tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}}-\sqrt{\ell(\ell+1)}-\frac{1}{2}\Big)\\
&+[\mathrm{Error}^B+\mathrm{Error}^C-\mathrm{Error}^D]\ .
\end{aligned}\tag{64}$$

Here we have used the fact that $\big(-V_\ell(x)\big)_+^{3/2}\equiv 0$ and $\big(-V_\ell(x)\big)_+^{-1/2}\equiv 0$ for $\ell\geq\Omega$; and that

$$\big(-V_\ell^c(x)\big)_+^{3/2}\equiv 0\quad\text{and}\quad\big(-V_\ell^c(x)\big)_+^{-1/2}\equiv 0\quad\text{for}\quad\ell\geq\Omega_c\ .$$

From (59 bis), (61), (63), we have

$$\big|[\mathrm{Error}^B+\mathrm{Error}^C-\mathrm{Error}^D]\big|\leq C\,Z^{\frac{8}{5}+2\cdot 10^{-9}}\ .\tag{65}$$

It is convenient to write (64) in a different form.

Fix a function $\varphi(x)$ equal to 1 for $x\geq 2\cdot Z^{-3/5}$, equal to zero for $x\leq Z^{-3/5}$, and satisfying the estimates

$$\Big|\Big(\frac{d}{dx}\Big)^\alpha\varphi(x)\Big|\leq C_\alpha x^{-\alpha}\quad\text{for}\quad x\in(0,\infty)\ ,\alpha\geq 0\ .\tag{66}$$

In view of (3), the expressions in curly brackets in (64) are supported in $\{x>2Z^{-3/5}\}$, where $\varphi\equiv 1$. Hence we may replace dx by $\varphi(x)dx$ in the integrals in (64). Therefore, (64), (65) may be rewritten as follows.

$$\operatorname{sneg}(H)-\operatorname{sneg}(H_c)=X-X_c+Y-Y_c+W-W_c+\mathrm{Error}^E\ ,\tag{67}$$

with

(68) $$X = -\frac{2}{3\pi}\sum_{\ell\geq 0}(2\ell+1)\int_0^\infty \big(-V_\ell(x)\big)_+^{3/2}\varphi(x)dx$$

(69) $$X_c = -\frac{2}{3\pi}\sum_{\ell\geq 0}(2\ell+1)\int_0^\infty \big(-V_\ell^c(x)\big)_+^{3/2}\varphi(x)dx$$

(70) $$Y = \frac{1}{24\pi}\sum_{\ell > Z^{10^{-9}}}(2\ell+1)\int_0^\infty V_\ell''(x)\cdot\big(-V_\ell(x)\big)_+^{-1/2}\varphi(x)dx$$

(71) $$Y_c = \frac{1}{24\pi}\sum_{\ell > Z^{10^{-9}}}(2\ell+1)\int_0^\infty V_\ell^{c\,\prime\prime}(x)\cdot\big(-V_\ell^c(x)\big)_+^{-1/2}\varphi(x)dx$$

(72) $$W = \pi\sum_{Z^{10^{-9}}<\ell<\Omega}\frac{(2\ell+1)}{n_\ell}\tilde{\chi}(\phi_\ell)$$

(73) $$W_c = \sum_{Z^{10^{-9}}<\ell<\Omega_c}(2\ell+1)\cdot\frac{2E_0^{3/2}}{Z}\tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}}-\sqrt{\ell(\ell+1)}-\frac{1}{2}\Big)$$

(74) $$|\mathrm{Error}^E| < C\,Z^{\frac{8}{5}+2\cdot 10^{-9}}\ .$$

In order to understand X, X_c, Y, Y_c, we study the expressions

(75) $$X(\theta, W) = \sum_{\ell\geq 0}(2\ell+1)\int_{-\infty}^\infty\Big(\frac{W(x)-\ell(\ell+1)}{x^2}\Big)_+^{3/2}\theta(x)dx \qquad \text{and}$$

(76)
$$Y(\theta, W) = \sum_{\ell > Z^{10^{-9}}}(2\ell+1)\int_{-\infty}^\infty\Big(-\big[\frac{W(x)}{x^2}\big]''+\frac{6\ell(\ell+1)}{x^4}\Big)\cdot\Big(\frac{W(x)-\ell(\ell+1)}{x^2}\Big)_+^{-1/2}\theta(x)dx\ .$$

Here we assume $\theta(x)$ is supported in $|x-x_0|\leq B$ and satisfies

(76bis) $$\Big|\Big(\frac{d}{dx}\Big)^\alpha\theta\Big|\leq C_\alpha B^{-\alpha}\ .$$

Regarding $W(x)$, we assume

$$(77)\qquad \left|\left(\frac{d}{dx}\right)^{\alpha} W\right| \le C_\alpha \mathcal{S} B^{-\alpha} \quad \text{for } |x-x_0|\le B \qquad \text{and either}$$

$$(78)\qquad |W'(x)| > c\mathcal{S}B^{-1} \quad \text{for} \quad |x-x_0|\le B \ , \ \text{or else}$$

$$(79)\qquad W'(x_0)=0 \quad \text{and} \quad -W''(x) > c\mathcal{S}B^{-2} \quad \text{for } |x-x_0|\le B \ .$$

We assume $\mathcal{S}\ge 1$. Later, we will write X and X_c as sums of $X(\theta_\nu, W)$, and similarly write Y, Y_c as sums of $Y(\theta_\nu, W)$ for suitable θ_ν, W. To understand (75), (76), we first study the functions

$$(80)\qquad F(\xi,\theta,W) = \int_{-\infty}^{\infty} \big(W(x)-\xi\big)_+^{3/2}\theta(x)dx \qquad \text{and}$$

$$(81)\qquad G(\xi,\theta,W) = \int_{-\infty}^{\infty} \big(W(x)-\xi\big)_+^{-1/2}\theta(x)dx$$

under assumptions (76 bis), (77), and either (78) or (79). Our basic result on F, G is as follows.

Lemma 9. *If (78) holds, then*

$$(82)\qquad \left|\left(\frac{d}{d\xi}\right)^{m} F(\xi,\theta,W)\right| \le C'_m(\mathcal{S}^{3/2}B)\mathcal{S}^{-m} \quad \textit{and}$$

$$(83)\qquad \left|\left(\frac{d}{d\xi}\right)^{m} G(\xi,\theta,W)\right| \le C'_m(\mathcal{S}^{-1/2}B)\mathcal{S}^{-m}$$

for $|\xi| < C\mathcal{S}$. *If instead (79) holds, then (82) and (83) are valid for* $-C\mathcal{S} < \xi < W(x_0)$. *The* C'_m *depend only on the constants* C_α *in (76 bis), (77), on* c *in (78), (79), and on* C *in the bounds for* ξ. *These conclusions do not require the assumption* $\mathcal{S}\ge 1$.

Proof. After rescaling, we may take $\mathcal{S}=B=1$. Suppose first that (78) holds. We may suppose $W'(x) > c$ in $\{|x-x_0|\le 1\}$. (Otherwise, $-W'(x) > c$, and we change variable from x to $-x$ without changing F, G.) Change variable from x to $y = W(x)$. The image of $\{|x - x_0| \leq 1\}$ is an interval $[y_{\min}, y_{\max}]$ with $|y_{\min}|, |y_{\max}| < C$, $|y_{\max} - y_{\min}| > c$. In terms of y, we have $\theta(x)dx = \tilde{\theta}(y)dy$ with $\tilde{\theta} \in C_0^\infty(y_{\min}, y_{\max})$ and the C^∞ seminorms of $\tilde{\theta}$ bounded a-priori in terms of the constants in (76 bis), (77), (78). In terms of y, the integrals defining F, G become

$$F(\xi, \theta, W) = \int_{-\infty}^{\infty} (y - \xi)_+^{3/2} \tilde{\theta}(y) dy = \int_0^\infty t^{3/2} \tilde{\theta}(\xi + t) dt \tag{84}$$

and

$$G(\xi, \theta, W) = \int_{-\infty}^{\infty} (y - \xi)_+^{-1/2} \tilde{\theta}(y) dy = \int_0^\infty t^{-1/2} \tilde{\theta}(\xi + t) dt \ . \tag{85}$$

If $|\xi| \leq C$, then $\tilde{\theta}(\xi + t) \equiv 0$ for $t > C' = y_{\max} + C$. Hence the t-integrals in (84), (85) may be taken over $(0, C')$ instead of $(0, \infty)$, without changing the value of the integrals.

Thus, for $|\xi| \leq C$ we have

$$F(\xi, \theta, W) = \int_0^{C'} t^{3/2} \tilde{\theta}(\xi + t) dt \qquad \text{and} \tag{86}$$

$$G(\xi, \theta, W) = \int_0^{C'} t^{-1/2} \tilde{\theta}(\xi + t) dt \ . \tag{87}$$

Since the constant C' and the C^∞-seminorms of $\tilde{\theta}$ are bounded a-priori in terms of the constants in (76 bis), (77), (78), the formulas (86) and (87) imply trivially the conclusion of Lemma 9.

On the other hand, assume (76 bis), (77) and (79). Then there is a smooth function $y(x)$ defined on $\{|x - x_0| \leq 1\}$ with $W(x) = W(x_0) - (y(x))^2$ and $y'(x) > c > 0$. The C^∞ seminorms of $y(x)$ are bounded a-priori in terms of the constants in (76 bis), (77), (79); and similarly, the lower bound c for $y'(x)$ is bounded below a-priori. Again we change variable from x to $y = y(x)$ in the definitions of F, G. We have $\theta(x)dx = \tilde{\theta}(y)dy$ for a function $\tilde{\theta}$ whose C^∞ seminorms are bounded a-priori, and supported in $[y_{\min}, y_{\max}]$ with $|y_{\min}|$, $|y_{\max}|$ bounded a-priori. Hence,

$$F(\xi,\theta,W) = \int_{-\infty}^{\infty} \big([W(x_0)-\xi]-y^2\big)_+^{3/2}\tilde{\theta}(y)dy \qquad \text{and} \tag{88}$$

$$G(\xi,\theta,W) = \int_{-\infty}^{\infty} \big([W(x_0)-\xi]-y^2\big)_+^{-1/2}\tilde{\theta}(y)dy \ . \tag{89}$$

Since $\tilde{\theta}$ is C^∞, we can write $\tilde{\theta}(y) = \theta_1(y^2) + y\theta_2(y^2)$, with the C^∞-seminorms of θ_1, θ_2 bounded a-priori. We substitute this in (88), (89), and note that the θ_2-term may be dropped, since it contributes the integral of an odd function. Thus

$$F(\xi,\theta,W) = \int_{-\infty}^{\infty} \big([W(x_0)-\xi]-y^2\big)_+^{3/2}\theta_1(y^2)dy \qquad \text{and}$$
$$G(\xi,\theta,W) = \int_{-\infty}^{\infty} \big([W(x_0)-\xi]-y^2\big)_+^{-1/2}\theta_1(y^2)dy \ .$$

If $\xi < W(x_0)$, then we may change variable to conclude that

$$F(\xi,\theta,W) = \int_{-1}^{1} (1-t^2)^{3/2}\theta_1(t^2[W(x_0)-\xi])dt \cdot [W(x_0)-\xi]^2$$
$$G(\xi,\theta,W) = \int_{-1}^{1} (1-t^2)^{-1/2}\theta_1(t^2[W(x_0)-\xi])dt \ .$$

Evidently, these two integrals are smooth functions on $\{|\xi| < C\}$, with C^∞ seminorms bounded a-priori. Hence the conclusion of Lemma 9 holds under the assumptions (76 bis), (77), (79). The proof of Lemma 9 is complete. ■

Next suppose $\theta \in C_0^\infty(|x-x_0| \le cx_0)$ with $0 < c < 1/2$ and

$$\Big|\Big(\frac{d}{dx}\Big)^\alpha \theta\Big| \le C_\alpha x_0^{-\alpha} \ . \tag{90}$$

Suppose also

$$\Big|\Big(\frac{d}{dx}\Big)^\alpha W\Big| \le C_\alpha \mathcal{S} x_0^{-\alpha} \quad \text{for } |x-x_0| \le cx_0 \ , \tag{91}$$

and either

$$|W'| > c'\mathcal{S}x_0^{-1} \quad \text{for} \quad |x - x_0| \leq cx_0 \; , \tag{92}$$

or else

$$W(x_0) > 0 \; , W'(x_0) = 0 \quad \text{and} \quad - W'' > c'\mathcal{S}x_0^{-2} \quad \text{for } |x - x_0| \leq cx_0 \; . \tag{93}$$

We assume also $\mathcal{S} \geq 1$.

Define

$$\mathcal{F}(\xi) = \int_0^\infty \Big(\frac{W(x) - \xi}{x^2}\Big)_+^{3/2} \theta(x) dx \qquad \text{and} \tag{94}$$

$$\mathcal{G}(\xi) = \int_0^\infty \Big(-[\frac{W(x)}{x^2}]'' + \frac{6\xi}{x^4}\Big) \cdot \Big(\frac{W(x) - \xi}{x^2}\Big)_+^{-1/2} \theta(x) dx \; . \tag{95}$$

Set $\theta_1(x) = \frac{x_0^3 \theta(x)}{x^3}$ and $\theta_2(x) = \frac{x[\frac{W(x)}{x^2}]'' \theta(x)}{x_0^{-3}\mathcal{S}}$. Both θ_1 and θ_2 satisfy the hypotheses of Lemma 9, with $B = cx_0$. (To see this, for θ_2, note that $x[\frac{W(x)}{x^2}]'' =$ (const) $x^{-3}W(x)+$ (const)$x^{-2}W'(x)+$ (const) $x^{-1}W''(x)$, so that $\big(\frac{d}{dx}\big)^\alpha \big\{x\big[\frac{W(x)}{x^2}\big]''\big\}$ is a sum of terms $x^{-a}\big(\frac{d}{dx}\big)^b W$ with $a + b = \alpha + 3$. Hence $\big|\big(\frac{d}{dx}\big)^\alpha \{x[\frac{W(x)}{x^2}]''\}\big| \leq C_\alpha \mathcal{S} x_0^{-3-\alpha}$ in supp θ, from which one verifies the estimate (76 bis) for θ_2.)

Immediately from the definitions (80), (81), (94), (95) we have

$$\mathcal{F}(\xi) = x_0^{-3} F(\xi, \theta_1, W) \quad \text{and} \tag{96}$$

$$\mathcal{G}(\xi) = -x_0^{-3}\mathcal{S} \cdot G(\xi, \theta_2, W) + 6\xi x_0^{-3} G(\xi, \theta_1, W) \; . \tag{97}$$

The terms on the right are controlled by using Lemma 9, with $B = cx_0$. We deduce from (96), (97) and Lemma 9 that

$$\big|\big(\frac{d}{d\xi}\big)^m \mathcal{F}(\xi)\big| \leq C_m(\mathcal{S}^{3/2}x_0^{-2})\mathcal{S}^{-m} \quad \text{for } \xi \in \mathcal{J} \; , \quad \text{and} \tag{98}$$

$$(99) \qquad \left|\left(\frac{d}{d\xi}\right)^m \mathcal{G}(\xi)\right| \le C_m(\mathcal{S}^{1/2} x_0^{-2})\mathcal{S}^{-m} \quad \text{for } \xi \in \mathcal{J} \ , \quad \text{where}$$

$$(100) \qquad \mathcal{J} = \{|\xi| < C\mathcal{S}\} \text{ in case (92) holds ,}$$

$$(101) \qquad \mathcal{J} = \{-C\mathcal{S} < \xi < W(x_0)\} \text{ in case (93) holds .}$$

Next, set

$$(102) \qquad f(t) = (2t+1)\mathcal{F}(t(t+1)) = (2t+1)\int_0^\infty \left(\frac{W(x) - t(t+1)}{x^2}\right)_+^{3/2} \theta(x)dx$$

$$(103) \qquad g(t) = (2t+1)\mathcal{G}(t(t+1))$$
$$= (2t+1)\int_0^\infty \left(-\left[\frac{W(x)}{x^2}\right]'' + \frac{6t(t+1)}{x^4}\right) \cdot \left(\frac{W(x)-t(t+1)}{x^2}\right)_+^{-1/2} \theta(x)dx \ .$$

Comparing these definitions with (75), (76), we see that

$$(104) \qquad X(\theta, W) = \sum_{\ell \ge 0} f(\ell) \quad \text{and} \quad Y(\theta, W) = \sum_{\ell > Z^{10^{-9}}} g(\ell) \ .$$

Our next task is to estimate the derivatives of f and g. The derivative $(\frac{d}{dt})^k \mathcal{F}(t(t+1))$ is a sum of terms

$$(105) \qquad \left(\frac{d}{d\xi}\right)^m \mathcal{F}(\xi) \Big|_{\xi = t(t+1)} \cdot \prod_{\nu=1}^m \left(\frac{d}{dt}\right)^{k_\nu} \{t(t+1)\}$$
$$\text{with } k_\nu \ge 1 \text{ and } k_1 + \ldots + k_m = k \ .$$

We are interested in $t \in [0, t_{\max})$, with $t_{\max} = C\mathcal{S}^{1/2}$ if (92) holds, and $t_{\max} =$ the positive root of $t_{\max}(t_{\max}+1) = W(x_0)$ if (93) holds. For t in this interval we have $\xi = t(t+1) \in \mathcal{J}$, and $|(\frac{d}{dt})^{k_\nu}\{t(t+1)\}| \le C\mathcal{S}^{1-\frac{k_\nu}{2}}$, since $|t| \le C\mathcal{S}^{1/2}$. Hence by (98), the term (105) is dominated by

$$C(\mathcal{S}^{3/2} x_0^{-2})\mathcal{S}^{-m} \cdot \prod_{\nu=1}^m \mathcal{S}^{1-\frac{k_\nu}{2}} = C(\mathcal{S}^{3/2} x_0^{-2})\mathcal{S}^{-\frac{k}{2}} \ .$$

Therefore,

$$\Big|\Big(\frac{d}{dt}\Big)^k \mathcal{F}(t(t+1))\Big| \le C_k(\mathcal{S}^{3/2}x_0^{-2})\mathcal{S}^{-k/2} \quad \text{for } t \in [0, t_{\max}) \ . \tag{106}$$

Similarly, using (99) instead of (98), we find that

$$\Big|\Big(\frac{d}{dt}\Big)^k \mathcal{G}(t(t+1))\Big| \le C_k(\mathcal{S}^{1/2}x_0^{-2})\mathcal{S}^{-k/2} \text{ for } t \in [0, t_{\max}) \ . \tag{107}$$

Also, $|(\frac{d}{dt})^k(2t+1)| \le C\mathcal{S}^{1/2-k/2}$ for $t \in [0, t_{\max})$, since $t_{\max} < C\mathcal{S}^{1/2}$. Combining this with (106), (107) and recalling the definitions (102), (103) of $f(t)$, $g(t)$, we obtain

$$\Big|\Big(\frac{d}{dt}\Big)^k f(t)\Big| \le C_k(\mathcal{S}^2 x_0^{-2})\mathcal{S}^{-k/2} \quad \text{for } t \in [0, t_{\max}) \ , \quad \text{and} \tag{108}$$

$$\Big|\Big(\frac{d}{dt}\Big)^k g(t)\Big| \le C_k(\mathcal{S} x_0^{-2})\mathcal{S}^{-k/2} \quad \text{for } t \in [0, t_{\max}) \ . \tag{109}$$

If $t \ge t_{\max}$, then $\frac{W(x)-t(t+1)}{x^2} \le 0$ in supp θ, so that $f(t) = g(t) = 0$ by definition (102), (103). Thus, (104) may be rewritten as

$$X(\theta, W) = \sum_{\ell \in [0, t_{\max}) \cap \mathbb{Z}} f(\ell) \tag{110}$$

$$Y(\theta, W) = \sum_{\ell \in (Z^{10^{-9}}, t_{\max}) \cap \mathbb{Z}} g(\ell) \ . \tag{111}$$

We compute $X(\theta, W)$ using (108), (110) and the lemma on Riemann sums. In that lemma, we take $a = 0$, $b = t_{\max} - \varepsilon$, and let $\varepsilon \to 0+$. Thus,

$$\begin{aligned} X(\theta, W) = \int_0^{t_{\max}} f(t)dt + \lim_{b \to t_{\max}-} \Big\{-f(b)\chi_-(b) + \frac{1}{2}f'(b)\tilde{\chi}(b)\Big\} \\ - f(0)\chi_+(0) - \frac{1}{2}f'(0)\tilde{\chi}(0) + \text{ Error}_X \ , \text{ with} \\ |\text{Error}_X| \le C(\mathcal{S}^2 x_0^{-2}) \cdot \mathcal{S}^{-1} + C_N(\mathcal{S}^2 x_0^{-2})\mathcal{S}^{-N/2} t_{\max} \ . \end{aligned} \tag{112}$$

Since $t_{\max} \le C\mathcal{S}^{1/2}$ in either case (92) or (93), it follows that

$$(113) \qquad |\mathrm{Error}_X| \le C\mathcal{S}x_0^{-2} \ .$$

Let us compute the terms on the right in (112). We have

$$(114) \quad \int_0^{t_{\max}} f(t)dt = \int_0^\infty f(t)dt \quad (\text{since } f(t) \equiv 0 \text{ for } t > t_{\max})$$
$$= \int_0^\infty (2t{+}1) \int_0^\infty \Big(\frac{W(x) - t(t+1)}{x^2}\Big)_+^{3/2} \theta(x)dxdt = \int_0^\infty \int_0^\infty \big(\frac{W(x) - \xi}{x^2}\big)_+^{3/2} \theta(x)dxd\xi$$
$$= \frac{2}{5}\int_0^\infty \big(\frac{W(x)}{x^2}\big)_+^{5/2} x^2\theta(x)dx \ .$$

Next, note that $f(b)$ and $f'(b)$ both tend to zero as $b \to t_{\max}-$. In fact, $f(b) = f'(b) = 0$ for b near $t_{\max} = C\mathcal{S}^{1/2}$, if (92) holds. If instead (93) holds, then for $\xi \to W(x_0)-$ we have

$$\mathcal{F}(\xi) = \int_0^\infty \big(\frac{W(x) - \xi}{x^2}\big)_+^{3/2} \theta(x)dx \to 0 \ , \quad \text{and}$$
$$\mathcal{F}'(\xi) = \ (\text{const}) \ \int_0^\infty (W(x) - \xi)_+^{1/2} \frac{\theta(x)}{x^3} dx \to 0 \ .$$

To see these equations, note that $(W(x) - \xi)_+$ is dominated by $C\mathcal{S}$ and supported in an interval about x_0 of length $O((W(x_0) - \xi)^{1/2})$. Thus $f(b), f'(b) \to 0$ as $b \to t_{\max}-$ in either case (92) or (93), since $f(b) = (2b{+}1)\mathcal{F}(b(b{+}1))$, and $b(b{+}1) \to W(x_0)-$. Hence

$$(115) \qquad \lim_{b \to t_{\max}-} \big\{-f(b)\chi_-(b) + \frac{1}{2}f'(b)\tilde{\chi}(b)\big\} = 0 \ .$$

Next, recall that $\chi_+(x) = k - x - \frac{1}{2}$ for the smallest integer $k \ge x$. Thus $\chi_+(0) = -\frac{1}{2}$, so

$$(116) \qquad -f(0)\chi_+(0) = +\frac{1}{2}f(0) = \frac{1}{2}\int_0^\infty \Big(\frac{W(x)}{x^2}\Big)_+^{3/2} \theta(x)dx \ .$$

Similarly, $\tilde{\chi}(0) = \min_{k \in \mathbb{Z}} \{|0 - k - 1/2|^2 - \frac{1}{12}\} = \frac{1}{4} - \frac{1}{12} = \frac{1}{6}$, and from the definition (102) we get

$$f'(0) = 2\int_0^\infty \Big(\frac{W(x)}{x^2}\Big)_+^{3/2} \theta(x)dx + \ (\text{const}) \ \int_0^\infty (W(x))_+^{1/2} \frac{\theta(x)}{x^3} dx \ .$$

The second term on the right is dominated by $\mathcal{S}^{1/2}x_0^{-2}$, so

(117) $$-\frac{1}{2}f'(0)\tilde{\chi}(0) = -\frac{1}{6}\int_0^\infty \Big(\frac{W(x)}{x^2}\Big)_+^{3/2}\theta(x)dx + \text{ Err }, \text{ with } |\text{Err}| \le C\mathcal{S}^{1/2}x_0^{-2} .$$

Putting (113)...(117) into (112), we see that

(118)
$$X(\theta, W) = \frac{2}{5}\int_0^\infty \Big(\frac{W(x)}{x^2}\Big)_+^{5/2} x^2\theta(x)dx + \frac{1}{3}\int_0^\infty \Big(\frac{W(x)}{x^2}\Big)_+^{3/2}\theta(x)dx + \text{ Error}'_X ,$$

with $|\text{Error}'_X| \le C\mathcal{S}x_0^{-2}$. (Recall $\mathcal{S} \ge 1$, so $\mathcal{S}^{1/2} \le \mathcal{S}$).

Similarly, we use (109), (111) and the lemma on Riemann sums to compute $Y(\theta, W)$. If $t_{\max} \le Z^{10^{-9}}$, then evidently $Y(\theta, W) = 0$ by (111). Suppose $t_{\max} > Z^{10^{-9}}$. For the interval $[a, b]$ in the Lemma on Riemann sums, we take $[Z^{10^{-9}} + \varepsilon, t_{\max} - \varepsilon]$ and let $\varepsilon \to 0+$. We obtain the following crude result, which is enough for our purposes.

(119) $$Y(\theta, W) = \int_{Z^{10^{-9}}}^{t_{\max}} g(t)dt + \text{ Error}_Y , \text{ with}$$

(120) $$|\text{Error}_Y| \le C(\mathcal{S}x_0^{-2}) + C_N(\mathcal{S}x_0^{-2})\mathcal{S}^{-N/2}t_{\max} \le C'\mathcal{S}x_0^{-2} ,$$

since $t_{\max} \le C\mathcal{S}^{1/2}$ as we noted before.

For $t > t_{\max}$ we have $g(t) \equiv 0$. Moreover, $\big|\int_0^{Z^{10^{-9}}} g(t)dt\big| \le C(\mathcal{S}x_0^{-2}) \cdot Z^{10^{-9}}$ by (109). Hence, (119) and (120) imply

(121) $$Y(\theta, W) = \int_0^\infty g(t)dt + \text{ Error}'_Y \text{ with } |\text{Error}'_Y| \le CZ^{10^{-9}}\mathcal{S}x_0^{-2} .$$

By definition (103), we have

(122)
$$\begin{aligned}\int_0^\infty g(t)dt &= \int_0^\infty (2t+1)\int_0^\infty \Big([-\frac{W(x)}{x^2}]'' + \frac{6t(t+1)}{x^4}\Big)\cdot\Big(\frac{W(x) - t(t+1)}{x^2}\Big)_+^{-1/2}\theta(x)dxdt \\ &= \int_0^\infty\int_0^\infty \Big([\frac{-W(x)}{x^2}]'' + \frac{6\xi}{x^4}\Big)\cdot\Big(\frac{W(x)-\xi}{x^2}\Big)_+^{-1/2}\theta(x)dxd\xi \\ &= \int_0^\infty [-\frac{W(x)}{x^2}]'' x\theta(x)\{\int_0^\infty (W(x)-\xi)_+^{-1/2}d\xi\}dx \\ &\quad + \int_0^\infty \frac{6\theta(x)}{x^3}\{\int_0^\infty \xi\cdot(W(x)-\xi)_+^{-1/2}d\xi\}dx .\end{aligned}$$

We evaluate the integrals in curly brackets:

$$\int_0^\infty \big(W(x)-\xi\big)_+^{-1/2} d\xi = 2\big(W(x)\big)_+^{1/2}\ , \text{ and}$$

$$\begin{aligned}\int_0^\infty \xi\big(W(x)-\xi\big)_+^{-1/2} d\xi &= \int_0^\infty \big[W(x)-(W(x)-\xi)\big]\cdot\big(W(x)-\xi\big)_+^{-1/2} d\xi \\ &= W(x)\cdot\int_0^\infty \big(W(x)-\xi\big)_+^{-1/2} d\xi - \int_0^\infty \big(W(x)-\xi\big)_+^{1/2} d\xi \\ &= W(x)\cdot 2\big(W(x)\big)_+^{1/2} - \frac{2}{3}\big(W(x)\big)_+^{3/2} = \frac{4}{3}\big(W(x)\big)_+^{3/2}\ .\end{aligned}$$

Hence (122) becomes

$$\int_0^\infty g(t)dt = 2\int_0^\infty \Big[\frac{-W(x)}{x^2}\Big]''\Big(\frac{W(x)}{x^2}\Big)_+^{1/2}\theta(x)x^2dx + 8\int_0^\infty \Big(\frac{W(x)}{x^2}\Big)_+^{3/2}\theta(x)dx\ .$$

Putting this into (121), we conclude that

$$\begin{aligned}Y(\theta,W) = 2\int_0^\infty \Big[-\frac{W(x)}{x^2}\Big]''\Big(\frac{W(x)}{x^2}\Big)_+^{1/2}\theta(x)x^2dx \\ +8\int_0^\infty \Big(\frac{W(x)}{x^2}\Big)_+^{3/2}\theta(x)dx + \text{ Error}'_Y\end{aligned} \tag{123}$$

with

$$\begin{aligned}|\text{Error}'_Y| \le CZ^{10^{-9}}\mathcal{S}x_0^{-2} \quad \text{if } t_{\max} > Z^{10^{-9}}\ ; \\ Y(\theta,W) = 0 \text{ if } t_{\max} \le Z^{10^{-9}}\ .\end{aligned} \tag{124}$$

We record our results (118), (123), (124) on $X(\theta,W)$, $Y(\theta,W)$ in the following statement.

Lemma 10. *Suppose $\theta(x)$, $W(x)$ are defined on $(0,\infty)$, with θ supported in $\{|x-x_0|\le cx_0\}$ $(0<c<1/2)$ and satisfying $\big|\big(\frac{d}{dx}\big)^\alpha\theta(x)\big| \le C_\alpha x_0^{-\alpha}$. Suppose also that $\mathcal{S}\ge 1$, $\big|\big(\frac{d}{dx}\big)^\alpha W\big| \le C_\alpha\mathcal{S}x_0^{-\alpha}$, and assume either*

(A) *$|W'(x)| > c'\mathcal{S}x_0^{-1}$ for $|x-x_0|\le cx_0$, in which case we set $t_{\max} = C\mathcal{S}^{1/2}$*

or

(B) *$W(x_0)>0$, $W'(x_0)=0$ and $-W''>c'\mathcal{S}x_0^{-2}$ for $|x-x_0|\le cx_0$ in which case we set $t_{\max}$ equal to the positive root of $t(t+1)=W(x_0)$.*

Then

$$X(\theta, W) = \sum_{\ell \geq 0} (2\ell+1) \int_0^\infty \Big(\frac{W(x) - \ell(\ell+1)}{x^2}\Big)_+^{3/2} \theta(x) dx$$

is given by

$$X(\theta, W) = \frac{2}{5} \int_0^\infty \Big(\frac{W(x)}{x^2}\Big)_+^{5/2} \theta(x) x^2 dx + \frac{1}{3} \int_0^\infty \Big(\frac{W(x)}{x^2}\Big)_+^{3/2} \theta(x) dx + \text{ Error}_X \ ,$$

with $|\text{Error}_X| \leq C\mathcal{S}x_0^{-2}$.

Also,

$$Y(\theta, W) = \sum_{\ell > Z^{10^{-9}}} (2\ell{+}1) \int_0^\infty \Big([-\frac{W(x)}{x^2}]'' {+} \frac{6\ell(\ell+1)}{x^4} \Big) {\cdot} \Big(\frac{W(x) - \ell(\ell+1)}{x^2} \Big)_+^{-1/2} \theta(x) dx$$

is given by

$$Y(\theta, W) = 2 \int_0^\infty \Big[-\frac{W(x)}{x^2} \Big]'' \Big(\frac{W(x)}{x^2}\Big)_+^{1/2} \theta(x) x^2 dx {+} 8 \int_0^\infty \Big(\frac{W(x)}{x^2}\Big)_+^{3/2} \theta(x) dx {+} \text{ Error}_Y$$

with

$$|\text{Error}_Y| \leq C Z^{10^{-9}} \mathcal{S} x_0^{-2} \ \textit{if}\ t_{\max} > Z^{10^{-9}} \ ;$$

$Y(\theta, W) = 0$ *if* $t_{\max} \leq Z^{10^{-9}}$.

We apply Lemma 10 to calculate the numbers X, Y, X_c, Y_c defined by equations (68)...(71). Define $W(x) = -x^2 V(x)$. Then:

(125) $$W(x) \sim \mathcal{S}(x) \equiv \min\{Zx, x^{-2}\} \quad \text{for } x \in (0, \infty)$$

(126) $$\big|\big(\frac{d}{dx}\big)^\alpha W(x)\big| \leq C_\alpha \mathcal{S}(x) x^{-\alpha}$$

(127) $W(x)$ has a single critical point at $x = \check{r} \sim Z^{-1/3}$, where

$$-W'' > c\mathcal{S}(\check{r})\check{r}^{-2} \ .$$

(128)

Outside any neighborhood $\{|x - \check{r}| < c_1 \check{r}\}$ we have $|W'(x)| > c_2 \mathcal{S}(x) x^{-1}$,

where c_2 depends on c_1 .

These properties are contained in Lemma 7 in the section on approximate T-F potentials.

Next, we use a partition of unity to write the function $\varphi(x)$ in (68)...(71) as a sum

$$\varphi(x) = \sum_\nu \theta_\nu(x) + \theta_{\text{far}}(x) \text{ , with the following properties .} \tag{129}$$

$$\text{Each } \theta_\nu(x) \text{ is supported in } \{|x - x_\nu| < cx_\nu\} \text{ for a small constant } c \text{ .} \tag{130}$$

$$\left|\left(\frac{d}{dx}\right)^\alpha \theta_\nu(x)\right| \le C_\alpha x_\nu^{-\alpha} \text{ .} \tag{131}$$

$$\text{Each } x_\nu \text{ lies between } cZ^{-3/5} \text{ and } C_1 Z^{-10^{-9}} \ (C_1 = \text{ large const.}) \tag{132}$$

$$\text{In each interval } [2^{-(k+1)}, 2^{-k}] \text{ there are at most } C \text{ of the } x_\nu \text{ .} \tag{133}$$

$$\theta_{\text{far}}(x) \text{ is supported in } [\tfrac{1}{2} C_1 Z^{-10^{-9}}, \infty) \text{ .} \tag{134}$$

$$|\theta_{\text{far}}(x)| \le C \text{ .} \tag{135}$$

(Recall that φ is supported in $\{x > cZ^{-3/5}\}$.)

By definitions (68), (70) and the definition of $X(\theta, W)$, $Y(\theta, W)$ in Lemma 10, we have

$$X = -\frac{2}{3\pi} X(\varphi, W) = -\frac{2}{3\pi} \sum_\nu X(\theta_\nu, W) - \frac{2}{3\pi} X(\theta_{\text{far}}, W) \text{ , and} \tag{136}$$

$$Y = \frac{1}{24\pi} Y(\varphi, W) = \frac{1}{24\pi} \sum_\nu Y(\theta_\nu, W) + \frac{1}{24\pi} Y(\theta_{\text{far}}, W) \text{ .} \tag{137}$$

For $\ell > Z^{10^{-9}}$, we have $\left(-V_\ell(x)\right)_+^{-1/2}$ supported in $[x_{\text{left}}(\ell), x_{\text{rt}}(\ell)]$. This interval is disjoint from the support of θ_{far}, by virtue of (134) and the fact that $x_{\text{rt}}(\ell) \sim \frac{1}{\ell}$.

(Here it is important to take the constant C_1 in (134) large enough). Consequently, $\int_0^\infty V_\ell''(x)\big(-V_\ell(x)\big)_+^{-1/2}\theta_{\text{far}}(x)dx = 0$ for $\ell > Z^{10^{-9}}$, so that

$$Y(\theta_{\text{far}}, W) = 0 \; . \tag{138}$$

To estimate $X(\theta_{\text{far}}, W)$, we use the same observations as in (138) to see that $\int_0^\infty \big(-V_\ell(x)\big)_+^{3/2}\theta_{\text{far}}(x)dx = 0$ for $\ell > Z^{10^{-9}}$. Therefore,

$$\begin{aligned}|X(\theta_{\text{far}}, W)| &= \Big| \sum_{0\le \ell\le Z^{10^{-9}}} (2\ell+1)\int_0^\infty \big(-V_\ell(x)\big)_+^{3/2}\theta_{\text{far}}(x)dx\Big| \\ &\le CZ^{2\cdot 10^{-9}}\int_0^\infty \big(-V(x)\big)_+^{3/2}|\theta_{\text{far}}(x)|dx \le C'\Big(\int_{\frac{1}{2}C_1 Z^{-10^{-9}}}^\infty x^{-6}dx\Big)Z^{2\cdot 10^{-9}} \\ &\le Z^{10^{-8}} \; .\end{aligned} \tag{139}$$

To control $X(\theta_\nu, W)$ and $Y(\theta_\nu, W)$ we invoke Lemma 10.

For each ν, the functions θ_ν, W satisfy the hypotheses of Lemma 10, with $\mathcal{S} = \mathcal{S}(x_\nu)$ and $t_{\max} \sim \mathcal{S}^{1/2}(x_\nu)$. In fact, the hypothesis on supp θ_ν and the bounds assumed for $|(\frac{d}{dx})^\alpha\theta_\nu|$ and $|(\frac{d}{dx})^\alpha W|$ are contained in (130), (131) and (126). We have $\mathcal{S} = \mathcal{S}(x_\nu) \ge 1$, by (125), (132). We must show that (A) or (B) holds in the statement of Lemma 10. If $|x_\nu - \check{r}| > 2cx_\nu$ with c as in (130), then we take $x_0 = x_\nu$ in the statement of Lemma 10, and alternative (A) holds by virtue of (128). We have $t_{\max} \equiv C\mathcal{S}^{1/2}(x_\nu)$ in that case. If instead $|x_\nu - \check{r}| \le 2cx_\nu$, then we take $x_0 = \check{r}$ in the statement of Lemma 10, and we use there $10c$ in place of c. Alternative (B) holds in this case, by virtue of (126), (127) and the fact that $\mathcal{S} \equiv \mathcal{S}(x_\nu) \sim \mathcal{S}(\check{r}) \sim Z^{2/3}$. Moreover, $t_{\max}$ is defined in this case as the positive root of $t(t+1) = W(\check{r}) \sim \mathcal{S}(\check{r}) \sim Z^{2/3}$, so $t_{\max} \sim \mathcal{S}^{1/2}(x_\nu)$. Thus in either case, the hypotheses of Lemma 10 hold, with $\mathcal{S} = \mathcal{S}(x_\nu)$ and $t_{\max} \sim \mathcal{S}^{1/2}(x_\nu)$. Applying Lemma 10 and recalling that $V(x) = -\frac{W(x)}{x^2}$, we get:

(140)

$$X(\theta_\nu, W) = \frac{2}{5}\int_0^\infty \big(-V(x)\big)_+^{5/2}\theta_\nu(x)x^2dx + \frac{1}{3}\int_0^\infty \big(-V(x)\big)_+^{3/2}\theta_\nu(x)dx + \ \text{Error}_X(\nu)$$

with

$$(141) \qquad |\text{Error}_X(\nu)| \le C\mathcal{S}(x_\nu)\cdot x_\nu^{-2} \ ; \text{ and}$$

$$(142) \quad Y(\theta_\nu, W) = 2\int_0^\infty V''(x)\cdot\big(-V(x)\big)_+^{1/2}\theta_\nu(x)x^2dx + 8\int_0^\infty \big(-V(x)\big)_+^{3/2}\theta_\nu(x)dx + \text{ Error}_Y(\nu)$$

with

$$(143) \quad |\text{Error}_Y(\nu)| \le CZ^{10^{-9}}\mathcal{S}(x_\nu)x_\nu^{-2} \quad \text{if } t_{\max} > Z^{10^{-9}} \ ;$$
$$Y(\theta_\nu, W) = 0 \quad \text{if } t_{\max} \le Z^{10^{-9}} \ .$$

Here, $t_{\max}$ depends on ν and has the order of magnitude $t_{\max} \sim \mathcal{S}^{1/2}(x_\nu)$. In fact, (142) and (143) hold for all ν. To see this, suppose $t_{\max} \le Z^{10^{-9}}$. We have

$$V'' = \Big(-\frac{W(x)}{x^2}\Big)'' = O(\mathcal{S}(x_\nu)x_\nu^{-4}) \text{ in supp } \theta_\nu \ , \quad \text{and}$$
$$V = -\frac{W(x)}{x^2} = O(\mathcal{S}(x_\nu)x_\nu^{-2}) \text{ in supp } \theta_\nu \ , \text{ by (126) .}$$

Hence $\int_0^\infty V''(x)\cdot\big(-V(x)\big)_+^{1/2}\theta_\nu(x)x^2dx$ and $\int_0^\infty \big(-V(x)\big)_+^{3/2}\theta_\nu(x)dx$ are dominated by $C\mathcal{S}^{3/2}(x_\nu)\cdot x_\nu^{-2} \sim t_{\max}\mathcal{S}(x_\nu)x_\nu^{-2} \le Z^{10^{-9}}\mathcal{S}(x_\nu)\cdot x_\nu^{-2}$. Since also $Y(\theta_\nu, W) = 0$ in this case, (142) and (143) are obvious. Thus for all ν we have (140)...(143). Putting (139), (140), (141) into (136) we get

(144)
$$X = -\frac{4}{15\pi}\int_0^\infty \big(-V(x)\big)_+^{5/2}\big(\sum_\nu \theta_\nu(x)\big)x^2dx - \frac{2}{9\pi}\int_0^\infty \big(-V(x)\big)_+^{3/2}\big(\sum_\nu \theta_\nu(x)\big)dx + \text{Error}_X$$

with

$$(145) \quad |\text{Error}_X| \le CZ^{10^{-8}} + C\sum_\nu \mathcal{S}(x_\nu)x_\nu^{-2}$$
$$\le CZ^{10^{-8}} + C\sum_{cZ^{-3/5}\le x_\nu \le Z^{-1/3}} (Zx_\nu)\cdot x_\nu^{-2} + C\sum_{x_\nu > Z^{-1/3}} (x_\nu^{-2})x_\nu^{-2}$$
$$\le C'Z^{8/5} \ . \quad \text{(Here we used (132) and (133).)}$$

Since also $\varphi(x) = \sum_\nu \theta_\nu(x) + \theta_{\text{far}}(x)$, and

$$\Big|\int_0^\infty \big(-V(x)\big)_+^{5/2}\big(\theta_{\text{far}}(x)\big)x^2dx\Big| \le C\int_{\frac{1}{2}C_1 Z^{-10^{-9}}}^\infty (x^{-4})^{5/2}x^2dx \le C' Z^{10^{-6}}$$

$$\Big|\int_0^\infty \big(-V(x)\big)_+^{3/2}\big(\theta_{\text{far}}(x)\big)dx\Big| \le C\int_{\frac{1}{2}C_1 Z^{-10^{-9}}}^\infty (x^{-4})^{3/2}dx \le C' Z^{10^{-6}} \ ,$$

equations (144), (145) may be rewritten in the form

$$\text{(146)}\quad X = -\frac{4}{15\pi}\int_0^\infty \big(-V(x)\big)_+^{5/2}\varphi(x)x^2dx - \frac{2}{9\pi}\int_0^\infty \big(-V(x)\big)_+^{3/2}\varphi(x)dx + \text{Error}_X$$

with

$$\text{(147)}\qquad |\text{Error}_X| \le C\,Z^{8/5} \ .$$

Thus we have computed X. Similarly, we compute Y by putting (138), (142), (143) into (137). Thus, we obtain

(148)

$$Y = \frac{1}{12\pi}\int_0^\infty V''(x)\big(-V(x)\big)_+^{1/2}\Big(\sum_\nu \theta_\nu(x)\Big)x^2dx + \frac{1}{3\pi}\int_0^\infty \big(-V(x)\big)_+^{3/2}\Big(\sum_\nu \theta_\nu(x)\Big)dx + \text{Error}_Y \ , \quad \text{with}$$

$$\text{(149)}\qquad |\text{Error}_Y| \le C\,Z^{10^{-9}}\sum_\nu \mathcal{S}(x_\nu)x_\nu^{-2} \le C' Z^{8/5+10^{-9}} \ .$$

(The last inequality follows from the intermediate steps in (145).) As before, we use $\varphi(x) = \sum_\nu \theta_\nu(x) + \theta_{\text{far}}(x)$ and

$$\Big|\int_0^\infty V''(x)\cdot\big(-V(x)\big)_+^{1/2}\theta_{\text{far}}(x)x^2dx\Big| \le C\int_{\frac{1}{2}C_1 Z^{-10^{-9}}}^\infty x^{-6}(x^{-4})^{1/2}x^2dx \le C' Z^{10^{-6}}$$

$$\Big|\int_0^\infty \big(-V(x)\big)_+^{3/2}\theta_{\text{far}}(x)dx\Big| \le C\int_{\frac{1}{2}C_1 Z^{-10^{-9}}}^\infty (x^{-4})^{3/2}dx \le C' Z^{10^{-6}}$$

to rewrite (148), (149) in the form

(150)

$$Y = \frac{1}{12\pi}\int_0^\infty V''(x)\cdot\big(-V(x)\big)_+^{1/2}\varphi(x)x^2dx + \frac{1}{3\pi}\int_0^\infty \big(-V(x)\big)_+^{3/2}\varphi(x) + \text{Error}_Y$$

with

$$|\mathrm{Error}_Y| \leq C\, Z^{\frac{8}{5}+10^{-9}} \ . \tag{151}$$

Thus, we have computed X and Y in (67)...(74).

Next, we make an analogous computation of X_c, Y_c, defined by (69), (71) in terms of the Coulomb potential $V_c(x) = E_0 - \frac{Z}{x}$. As in (125)...(128), we now define $W_c(x) = -x^2 V_c(x) = Zx - E_0 x^2$. The analogues of (125)...(128) are as follows. Set $\mathcal{S}_c(x) = Zx$. Then:

$$\left|\left(\frac{d}{dx}\right)^{\alpha} W_c(x)\right| \leq C_\alpha \mathcal{S}_c(x) x^{-\alpha} \quad \text{for } 0 < x < \frac{20\, Z}{E_0} \tag{152}$$

(153) $W_c(x)$ has a single critical point at $x = \check{r}_c = \dfrac{Z}{2E_0} \sim Z^{-1/3}$,

$$\text{where } -W'' > c\mathcal{S}_c(\check{r}_c)\check{r}_c^{-2} \text{ and } W \sim \mathcal{S}_c(\check{r}_c) \ .$$

(154) For $x \in (0, \dfrac{10\, Z}{E_0})$ outside the interval $\{|x - \check{r}_c| < c_1 \check{r}_c\}$ we have

$$|W_c'(x)| > c_2 \mathcal{S}_c(x) x^{-1} \ , \text{ where } c_2 \text{ depends on } c_1 \ .$$

$$W_c(x) < 0 \quad \text{for } x \geq \frac{2Z}{E_0} \sim Z^{-1/3} \ . \tag{155}$$

We again use the decomposition (129) of φ. As in (136), (137), we have

$$X_c = -\frac{2}{3\pi} \sum_\nu X(\theta_\nu, W_c) - \frac{2}{3\pi} X(\theta_{\mathrm{far}}, W_c) \quad \text{and} \tag{156}$$

$$Y_c = \frac{1}{24\pi} \sum_\nu Y(\theta_\nu, W_c) + \frac{1}{24\pi} Y(\theta_{\mathrm{far}}, W_c) \ . \tag{157}$$

Since $W_c(x) < 0$ in supp θ_{far} by (134), (155), it follows immediately from the definitions of $X(\theta, W)$ and $Y(\theta, W)$ that

$$X(\theta_{\mathrm{far}}, W_c) = Y(\theta_{\mathrm{far}}, W_c) = 0 \ . \tag{158}$$

Similarly,

(159) $$X(\theta_\nu, W_c) = Y(\theta_\nu, W_c) = 0 \quad \text{if } x_\nu > 10\frac{Z}{E_0}\ .$$

For $x_\nu \le 10\frac{Z}{E_0}$, we can read off $X(\theta_\nu, W_c)$ and $Y(\theta_\nu, W_c)$ from Lemma 10, as in (139)…(143). In fact, the hypotheses of Lemma 10 hold here for θ_ν, W_c, with $\mathcal{S} = \mathcal{S}_c(x_\nu)$ and $t_{\max} \sim \mathcal{S}_c^{1/2}(x_\nu)$. To check the hypotheses of Lemma 10, we argue as in the paragraphs following (139), with (152)…(154) playing the role of (125)…(128). Note that $t_{\max} \sim (Zx_\nu)^{1/2} > Z^{10^{-9}}$ for all the x_ν. Hence Lemma 10 yields the following results analogous to (140)…(143).

If $x_\nu \le 10\frac{Z}{E_0}$, then

(160)
$$X(\theta_\nu, W_c) = \frac{2}{5}\int_0^\infty \big(-V_c(x)\big)_+^{5/2}\theta_\nu(x)x^2dx + \frac{1}{3}\int_0^\infty \big(-V_c(x)\big)_+^{3/2}\theta_\nu(x)dx + \text{Error}_X^c(\nu)$$

with

(161) $$|\text{Error}_X^c(\nu)| \le C\mathcal{S}_c(x_\nu)\cdot x_\nu^{-2}\ , \quad \text{and}$$

(162)
$$Y(\theta_\nu, W_c) = 2\int_0^\infty V_c''(x)\cdot\big(-V_c(x)\big)_+^{1/2}\theta_\nu(x)x^2dx + 8\int_0^\infty \big(-V_c(x)\big)_+^{3/2}\theta_\nu(x)dx + \text{Error}_Y^c(\nu)$$

with

(163) $$|\text{Error}_Y^c(\nu)| \le CZ^{10^{-9}}\mathcal{S}_c(x_\nu)\cdot x_\nu^2\ .$$

If instead $x_\nu > \frac{10\,Z}{E_0}$, then $V_c > 0$ on supp θ_ν by (130), (155). Therefore (160), (162) hold with $\text{Error}_X^c(\nu) = \text{Error}_Y^c(\nu) = 0$, by virtue of (159). Hence, as in the proof of (144), (145), we get

(164)
$$X_c = -\frac{4}{15\pi}\int_0^\infty \big(-V_c(x)\big)_+^{5/2}\Big(\sum_\nu \theta_\nu(x)\Big)x^2dx - \frac{2}{9\pi}\int_0^\infty \big(-V_c(x)\big)_+^{3/2}\Big(\sum_\nu \theta_\nu(x)\Big)dx + \text{Error}_X^c$$

and

(165) $$|\text{Error}_X^c| \le C \sum_{x_\nu < \frac{10Z}{E_0}} \mathcal{S}_c(x_\nu) x_\nu^{-2} \le C' Z^{\frac{8}{5}} \ .$$

Since $V_c(x) > 0$ in supp θ_{far}, we have also

$$\int_0^\infty \big(-V_c(x)\big)_+^{5/2} (\theta_{\text{far}}(x)\big) x^2 dx = \int_0^\infty \big(-V_c(x)\big)_+^{3/2} (\theta_{\text{far}}(x)\big) dx = 0 \ ,$$

so that (164), (165) may be rewritten in the form

(166)
$$X_c = -\frac{4}{15\pi} \int_0^\infty \big(-V_c(x)\big)_+^{5/2} \varphi(x) x^2 dx - \frac{2}{9\pi} \int_0^\infty \big(-V_c(x)\big)_+^{3/2} \varphi(x) dx + \ \text{Error}_X^c$$

with

(167) $$|\text{Error}_X^c| \le C Z^{\frac{8}{5}} \ .$$

Thus, we have succeeded in computing X_c. Similarly for Y_c, we obtain as in (148) the equation

$$Y_c = \frac{1}{12\pi} \int_0^\infty V_c'' \cdot \big(-V_c(x)\big)_+^{1/2} \big(\sum_\nu \theta_\nu(x)\big) x^2 dx + \frac{1}{3\pi} \int_0^\infty \big(-V_c(x)\big)_+^{3/2} \big(\sum_\nu \theta_\nu(x)\big) dx + \ \text{Error}_Y^c \ , \quad \text{with}$$

$$|\text{Error}_Y^c| \le C\, Z^{\frac{8}{5} + 10^{-9}} \ .$$

Again using the fact that $V_c(x) > 0$ in supp (θ_{far}), we can rewrite these equations in the form:

(168) $$Y_c = \frac{1}{12\pi} \int_0^\infty V_c''(x) \cdot \big(-V_c(x)\big)_+^{1/2} \varphi(x) x^2 dx + \frac{1}{3\pi} \int_0^\infty \big(-V_c(x)\big)_+^{3/2} \varphi(x) dx + \ \text{Error}_Y^c$$

with

(169) $$|\text{Error}_Y^c| \le C\, Z^{\frac{8}{5} + 10^{-9}} \ .$$

We have computed X, Y, X_c, Y_c in (67). Next we compute W_c, which is defined in (73). The function $\tilde{\chi}$ is Lipschitz continuous and periodic with period 1. Hence

$$\tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}} - \sqrt{\ell(\ell+1)} - \frac{1}{2}\Big) = \tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}} - [\ell + \frac{1}{2} + O(\ell^{-1})] - \frac{1}{2}\Big)$$

$$= \tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}} - \ell - 1\Big) + O(\ell^{-1}) = \tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}}\Big) + O(\ell^{-1}) \; .$$

Putting this into (73), we get

$$\text{(170)} \quad W_c = \sum_{Z^{10^{-9}} < \ell < \Omega_c} (2\ell+1) \cdot \frac{2E_0^{3/2}}{Z} \tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}}\Big) + \sum_{Z^{10^{-9}} < \ell < \Omega_c} (2\ell+1) \cdot \frac{2E_0^{3/2}}{Z} \cdot O(\ell^{-1})$$

$$= [\Omega_c^2 + O(\Omega_c)] \cdot \frac{2E_0^{3/2}}{Z} \tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}}\Big) + O(\Omega_c) \cdot \frac{E_0^{3/2}}{Z}$$

$$= \Omega_c^2 \cdot 2E_0^{3/2} Z^{-1} \tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}}\Big) + O(\Omega_c E_0^{3/2} Z^{-1}) \; .$$

Recall that Ω_c is defined as the positive root of $\Omega_c(\Omega_c+1) = \max_{x>0}(-x^2 V_c(x)) = \max_{x>0}(Zx - E_0 x^2) = \frac{1}{4}\frac{Z^2}{E_0}$. (The max. is attained at $x = \frac{1}{2}\frac{Z}{E_0}$). Thus, $\Omega_c^2 = \frac{1}{4}\frac{Z^2}{E_0} - \Omega_c$. Substituting this into (170), we get

$$W_c = (\frac{1}{4} Z^2 E_0^{-1}) \cdot 2E_0^{3/2} Z^{-1} \tilde{\chi}(\frac{Z}{2E_0^{1/2}}) + O(\Omega_c E_0^{3/2} Z^{-1}) \; ,$$

i.e.

$$\text{(171)} \qquad W_c = \frac{1}{2} Z E_0^{1/2} \tilde{\chi}(\frac{Z}{2E_0^{1/2}}) + \text{ Error}_W \; , \quad \text{with}$$

$$\text{(172)} \qquad |\text{Error}_W| \le C\, Z^{4/3} \; .$$

(Recall that $\Omega_c \sim Z^{+1/3}$, $E_0 \sim Z^{+4/3}$.)

We prepare to substitute our results on X, X_c, Y, Y_c, W_c into (67). First of all, (146), (147), (166), (167) together yield:

$$X - X_c = -\frac{4}{15\pi} \int_0^\infty \big[\big(-V(x)\big)_+^{5/2} - \big(-V_c(x)\big)_+^{5/2}\big] \varphi(x) x^2 dx$$

$$\text{(173)} \qquad - \frac{2}{9\pi} \int_0^\infty \big[\big(-V(x)\big)_+^{3/2} - \big(-V_c(x)\big)_+^{3/2}\big] \varphi(x) dx + \text{ Error}_X^*$$

with $|\text{Error}^*_X| \le C\, Z^{8/5}$. We can omit the factor $\varphi(x)$ in the two integrals in (173), since $V(x) = V_c(x)$ for $\varphi(x) \ne 1$ by virtue of (3) and the definition of φ. Therefore,

$$\begin{aligned} X - X_c = &-\frac{4}{15\pi}\int_0^\infty \left[\left(-V(x)\right)_+^{5/2} - \left(-V_c(x)\right)_+^{5/2}\right]x^2 dx \\ &- \frac{2}{9\pi}\int_0^\infty \left[\left(-V(x)\right)_+^{3/2} - \left(-V_c(x)\right)_+^{3/2}\right]dx + \text{Error}^*_X \ , \end{aligned} \tag{174}$$

with

$$|\text{Error}^*_x| \le C\, Z^{8/5} \ . \tag{175}$$

Similarly, combining (150), (151) with (168), (169) and dropping the factors $\varphi(x)$ from the resulting integrals, we find that

$$\begin{aligned} Y - Y_c = &\frac{1}{12\pi}\int_0^\infty \left[V''(x)\cdot\left(-V(x)\right)_+^{1/2} - V_c''(x)\cdot\left(-V_c(x)\right)_+^{1/2}\right]x^2 dx \\ &+ \frac{1}{3\pi}\int_0^\infty \left[\left(-V(x)\right)_+^{3/2} - \left(-V_c(x)\right)_+^{3/2}\right]dx + \text{Error}^*_Y \ , \end{aligned} \tag{176}$$

with

$$|\text{Error}^*_Y| \le C\, Z^{\frac{8}{5}+10^{-9}} \ . \tag{177}$$

Combining (174)...(177), we get

$$\begin{aligned} X - X_c + Y - Y_c = &-\frac{4}{15\pi}\int_0^\infty \left[\left(-V(x)\right)_+^{5/2} - \left(-V_c(x)\right)_+^{5/2}\right]x^2 dx \\ &+ \frac{1}{12\pi}\int_0^\infty \left[V''(x)\cdot\left(-V(x)\right)_+^{1/2} - V_c''(x)\cdot\left(-V_c(x)\right)_+^{1/2}\right]x^2 dx \\ &+ \frac{1}{9\pi}\int_0^\infty \left[\left(-V(x)\right)_+^{3/2} - \left(-V_c(x)\right)_+^{3/2}\right]dx + \text{Error}_F \end{aligned} \tag{178}$$

with

$$|\text{Error}_F| \le C\, Z^{\frac{8}{5}+10^{-9}} \ . \tag{179}$$

We can simplify the right-hand side of (178) by an elementary integration by parts. For $\tilde V(x)$ smooth on $(0,\infty)$, the function $\left(-\tilde V(x)\right)_+^{3/2}$ belongs to $C^1(0,\infty)$, so that

$$\int_{\varepsilon_1}^R \left(-\tilde V(x)\right)_+^{3/2} dx = x\cdot\left(-\tilde V(x)\right)_+^{3/2}\Big]_{\varepsilon_1}^R - \int_{\varepsilon_1}^R \frac{3}{2}\left(-\tilde V(x)\right)_+^{1/2}\cdot\left(-\tilde V'(x)\right)x dx \ .$$

We apply this to $\tilde{V} = V$ and to $\tilde{V} = V_c$. In either case, we may let $R \to \infty$, obtaining

$$\int_{\varepsilon_1}^{\infty} \big(-V(x)\big)_+^{3/2} dx = -\varepsilon_1 \big(-V(\varepsilon_1)\big)_+^{3/2} + \frac{3}{4} \int_{\varepsilon_1}^{\infty} \frac{2}{x} V'(x) \cdot \big(-V(x)\big)_+^{1/2} x^2 dx \quad \text{and}$$
$$\int_{\varepsilon_1}^{\infty} \big(-V_c(x)\big)_+^{3/2} dx = -\varepsilon_1 \big(-V_c(\varepsilon_1)\big)_+^{3/2} + \frac{3}{4} \int_{\varepsilon_1}^{\infty} \frac{2}{x} V_c'(x) \cdot \big(-V_c(x)\big)_+^{1/2} x^2 dx \; .$$

Subtracting and recalling that $V(x) = V_c(x)$ for $x \le \varepsilon_1$ (if we pick $\varepsilon_1 < Z^{-3/5}$ — see (3)), we get

$$\int_0^{\infty} \big[\big(-V(x)\big)_+^{3/2} - \big(-V_c(x)\big)_+^{3/2}\big] dx$$
$$= \frac{3}{4} \int_0^{\infty} \big[\frac{2}{x} V'(x) \cdot \big(-V(x)\big)_+^{1/2} - \frac{2}{x} V_c'(x) \cdot \big(-V_c(x)\big)_+^{1/2}\big] x^2 dx \; .$$

Putting this into (178), (179), we get

$$X - X_c + Y - Y_c$$
$$= -\frac{4}{15\pi} \int_0^{\infty} \big[\big(-V(x)\big)_+^{5/2} - \big(-V_c(x)\big)_+^{5/2}\big] x^2 dx$$
$$+ \frac{1}{12\pi} \int_0^{\infty} \big[\big(V''(x) + \frac{2}{x} V'(x)\big) \cdot \big(-V(x)\big)_+^{1/2} - \big(V_c''(x) + \frac{2}{x} V_c'(x)\big) \cdot \big(-V_c(x)\big)_+^{1/2}\big] x^2 dx$$
$$+ \text{ Error}_F \; , \quad \text{with Error}_F \text{ as in (178), (179)} \; .$$

For $V_c(x) = E_0 - \frac{Z}{x}$, we have $V_c''(x) + \frac{2}{x} V_c'(x) = 0$, so the preceding equation simplifies to

$$X - X_c + Y - Y_c$$
$$= -\frac{4}{15\pi} \int_0^{\infty} \big(-V(x)\big)_+^{5/2} x^2 dx + \frac{4}{15\pi} \int_0^{\infty} \big(-V_c(x)\big)_+^{5/2} x^2 dx$$
$$+ \frac{1}{12\pi} \int_0^{\infty} \big(V''(x) + \frac{2}{x} V'(x)\big) \cdot \big(-V(x)\big)_+^{1/2} x^2 dx + \text{ Error}_F \tag{180}$$

with Error_F as before.

Next we compute the term $\int_0^{\infty} \big(-V_c(x)\big)_+^{5/2} x^2 dx$ in (180). (We include details for the reader's convenience.) In the discussion of elementary integrals in the Review of Earlier Results, we saw that

$$\frac{1}{\pi} \int_0^{\infty} \big(\frac{Z}{x} - \frac{P}{x^2} - E\big)_+^{1/2} dx = \frac{Z}{2\sqrt{E}} - \sqrt{P} \quad \text{for } Z, E, P, Z^2 - 4EP > 0 \; . \tag{181}$$

In particular, this holds for all $E \in (0, E_0]$ when $Z, E_0, P, Z^2 - 4E_0P > 0$. Integrating (181) in E over $(0, E_0]$, we obtain

$$-\frac{2}{3\pi}\int_0^\infty \Big(\frac{Z}{x} - \frac{P}{x^2} - E_0\Big)_+^{3/2} dx + \frac{2}{3\pi}\int_0^\infty \Big(\frac{Z}{x} - \frac{P}{x^2}\Big)_+^{3/2} dx = ZE_0^{1/2} - P^{1/2}E_0 \ .$$

Hence,

(182)
$$-\frac{2}{3\pi}\int_0^\infty \Big(\frac{Z}{x} - \frac{P}{x^2} - E_0\Big)_+^{3/2} dx = ZE_0^{1/2} - P^{1/2}E_0 + G(Z,P) \ ,$$
$$\text{whenever } Z, E_0, P > 0 \quad \text{and} \quad P < Z^2/(4E_0) \ ,$$

for some function $G(Z,P)$. The left side of (182) tends to zero as E_0 approaches $Z^2/(4P)$ from below. Therefore, $G(Z,P) = P^{1/2}\cdot\big(\frac{Z^2}{4P}\big) - Z\cdot\big(\frac{Z^2}{4P}\big)^{1/2} = -\frac{Z^2}{4P^{1/2}}$, so that (182) becomes

(183)
$$-\frac{2}{3\pi}\int_0^\infty \Big(\frac{Z}{x} - \frac{P}{x^2} - E_0\Big)_+^{3/2} dx = ZE_0^{1/2} - E_0P^{1/2} - \frac{1}{4}Z^2P^{-1/2}$$
$$\text{for } Z, E_0, P > 0 \quad \text{and} \quad Z^2 - 4E_0P > 0 \ .$$

Integrating (183) in P over the interval $(0, \frac{Z^2}{4E_0})$ and noting that $(\frac{Z}{x} - \frac{P}{x^2} - E_0)_+^{5/2} \equiv 0$ when $P = \frac{Z^2}{4E_0}$, we find that

$$-\frac{4}{15\pi}\int_0^\infty \Big(\frac{Z}{x} - E_0\Big)_+^{5/2} x^2 dx = ZE_0^{1/2}\cdot\Big(\frac{Z^2}{4E_0}\Big) - \frac{2}{3}E_0\Big(\frac{Z^2}{4E_0}\Big)^{3/2} - \frac{1}{4}Z^2\cdot 2\Big(\frac{Z^2}{4E_0}\Big)^{1/2} \ ,$$

i.e.

$$-\frac{4}{15\pi}\int_0^\infty \big(-V_c(x)\big)_+^{5/2} x^2 dx = -\frac{1}{12}\ \frac{Z^3}{E_0^{1/2}} \ .$$

Putting this equation into (180), we obtain

$$\begin{aligned} &X - X_c + Y - Y_c \\ &= -\frac{4}{15\pi}\int_0^\infty \big(-V(x)\big)_+^{5/2} x^2 dx + \frac{1}{12\pi}\int_0^\infty \Big(V''(x) + \frac{2}{x}V'(x)\Big)\cdot\big(-V(x)\big)_+^{1/2} x^2 dx \\ &\qquad + \frac{1}{12}Z^3E_0^{-1/2} + \text{ Error}_F \ , \end{aligned}$$

with Error_F estimated by (179).

Combining this with the definition (72) of W and equations (171), (172) for W_c, we conclude that

$$(184)\quad X - X_c + Y - Y_c + W - W_c$$
$$= -\frac{4}{15\pi}\int_0^\infty \big(-V(x)\big)_+^{5/2} x^2 dx + \frac{1}{12\pi}\int_0^\infty \big(V''(x) + \frac{2}{x}V'(x)\big)\cdot\big(-V(x)\big)_+^{1/2} x^2 dx$$
$$+\pi \sum_{Z^{10^{-9}}<\ell<\Omega} \frac{(2\ell+1)}{n_\ell}\tilde{\chi}(\phi_\ell) + \frac{1}{12}Z^3 E_0^{-1/2} - \frac{1}{2}Z E_0^{1/2}\tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}}\Big)$$
$$+ \ \mathrm{Error}_G \ ,$$

with

$$(185)\qquad |\mathrm{Error}_G| \le C\, Z^{\frac{8}{5}+10^{-9}} \ .$$

Substituting (184), (185) into (67), and recalling (74), we obtain the formula:

$$(186)\quad \mathrm{sneg}(H) - \ \mathrm{sneg}(H_c)$$
$$= -\frac{4}{15\pi}\int_0^\infty \big(-V(x)\big)_+^{5/2} x^2 dx + \frac{1}{12\pi}\int_0^\infty \big(V''(x) + \frac{2}{x}V'(x)\big)\cdot\big(-V(x)\big)_+^{1/2} x^2 dx$$
$$+\pi \sum_{Z^{10^{-9}}<\ell<\Omega} \frac{(2\ell+1)}{n_\ell}\tilde{\chi}(\phi_\ell)$$
$$+\frac{1}{12}Z^3 E_0^{-1/2} - \frac{1}{2}Z E_0^{1/2}\tilde{\chi}\Big(\frac{Z}{2E_0^{1/2}}\Big) + \ \mathrm{Error}_H \ ,$$

with

$$(187)\qquad |\mathrm{Error}_H| \le C\, Z^{\frac{8}{5}+2\cdot 10^{-9}} \ .$$

Next we compute $\mathrm{sneg}(H_c)$. Recall that the eigenvalues of $H_c = -\Delta + E_0 - \frac{Z}{|x|}$ on $\mathbb{R}^3$ are given by $E_0 - \frac{Z^2}{4n^2}$ with multiplicity n^2 $(n = 1, 2, 3, \ldots)$. Therefore,

$$(188)\qquad \mathrm{sneg}(H_c) = \sum_{1\le n\le \frac{Z}{2E_0^{1/2}}} n^2\Big(E_0 - \frac{Z^2}{4n^2}\Big) = \sum_{1\le n\le \frac{Z}{2E_0^{1/2}}} \Big(E_0 n^2 - \frac{Z^2}{4}\Big) \ .$$

We evaluate the right-hand side of (188) by using the Lemma on Riemann sums, with

$$f(t) = E_0 t^2 - \frac{Z^2}{4}\ , \quad [a,b] = \Big[1, \frac{Z}{2E_0^{1/2}}\Big]\ , \quad \sigma(t) \equiv Z^2\ , \quad \tau(t) \equiv Z^{1/3}\ .$$

The hypotheses of the Lemma on Riemann Sums are easily verified, since $E_0 \sim Z^{4/3}$. Thus we obtain from (188) and the Lemma on Riemann sums:

$$(189)\quad \mathrm{sneg}(H_c) = \sum_{n\in\mathbb{Z}\cap[a,b]} f(n)$$
$$= \int_a^b f(t)dt - f(b)\chi_-(b) - f(a)\chi_+(a) + \frac{1}{2}f'(b)\tilde{\chi}(b) - \frac{1}{2}f'(a)\tilde{\chi}(a) + \text{ Error },$$
$$\text{with } |\text{Error}| \le C\frac{\sigma(a)}{\tau^2(a)} + C\frac{\sigma(b)}{\tau^2(b)} + C\int_a^b \sigma(t)\tau^{-100}(t)dt \sim Z^{4/3} .$$

We have

$$(190)\quad \int_a^b f(t)dt = \int_1^{Z/(2E_0^{1/2})} \big(E_0 t^2 - \frac{Z^2}{4}\big)dt$$
$$= \Big(\frac{1}{3}E_0\big[\frac{Z}{2E_0^{1/2}}\big]^3 - \frac{Z^2}{4}\cdot\big[\frac{Z}{2E_0^{1/2}}\big]\Big) - \Big(\frac{1}{3}E_0 - \frac{Z^2}{4}\Big)$$
$$= -\frac{1}{12}Z^3E_0^{-1/2} + \frac{Z^2}{4} + O(Z^{4/3}) ,$$

$$(191)\qquad f(b)\chi_-(b) = 0 , \quad \text{since} \quad f(b) = E_0\big(\frac{Z}{2E_0^{1/2}}\big)^2 - \frac{Z^2}{4} = 0$$

$$(192)\quad f(a)\chi_+(a) = \big(E_0 - \frac{Z^2}{4}\big)\chi_+(1) = \big(E_0 - \frac{Z^2}{4}\big)\cdot(-\frac{1}{2})$$
$$(\text{by definition of } \chi_+(-)) = +\frac{Z^2}{8} + O(Z^{4/3})$$

$$\frac{1}{2}f'(b)\tilde{\chi}(b) = \frac{1}{2}\cdot(2E_0 b)\tilde{\chi}(b) = \frac{1}{2}\cdot\big(2E_0\cdot\frac{Z}{2E_0^{1/2}}\big)\tilde{\chi}\big(\frac{Z}{2E_0^{1/2}}\big)$$
$$(193)\qquad = \frac{1}{2}ZE_0^{1/2}\tilde{\chi}\big(\frac{Z}{2E_0^{1/2}}\big)$$

$$(194)\qquad \frac{1}{2}f'(a)\tilde{\chi}(a) = \frac{1}{2}\cdot(2E_0)\tilde{\chi}(1) = O(Z^{4/3}) .$$

Putting (190)…(194) into (189), we find that

$$\mathrm{sneg}(H_c) = \Big(-\frac{1}{12}Z^3E_0^{-1/2} + \frac{Z^2}{4}\Big) - \big(\frac{Z^2}{8}\big) + \Big(\frac{1}{2}ZE_0^{1/2}\tilde{\chi}\big(\frac{Z}{2E_0^{1/2}}\big)\Big) + O(Z^{4/3})$$
$$= -\frac{1}{12}Z^3E_0^{-1/2} + \frac{Z^2}{8} + \frac{1}{2}ZE_0^{1/2}\tilde{\chi}\big(\frac{Z}{2E_0^{1/2}}\big) + O(Z^{4/3}) .$$

Adding this equation to (186) and recalling (187), we obtain our basic formula for $\mathrm{sneg}(H)$, namely

$$(195)\quad \mathrm{sneg}(H)$$
$$= -\frac{4}{15\pi}\int_0^\infty \big(-V(x)\big)_+^{5/2}x^2dx + \frac{Z^2}{8} + \frac{1}{12\pi}\int_0^\infty \big(V''(x)+\frac{2}{x}V'(x)\big)\cdot\big(-V(x)\big)_+^{1/2}x^2dx$$
$$+\pi \sum_{Z^{10^{-9}}<\ell<\Omega} \frac{(2\ell+1)}{n_\ell}\tilde{\chi}(\phi_\ell) + \text{ Error}_I\ ,$$

with

$$(196)\qquad |\text{Error}_I| \le C\, Z^{\frac{8}{5}+2\cdot 10^{-9}}\ .$$

These results hold under the assumptions (1), (2), (3) above, with ϕ_ℓ, n_ℓ given by (6) and (7).

It will be convenient to modify slightly the sum in (195). To do so, we give a lower bound for n_ℓ. Recall that $\{V_\ell(r)<0\} = (x_{\text{left}}(\ell), x_{\text{rt}}(\ell))$ with $x_{\text{left}}(\ell) \sim \frac{\ell^2}{Z}$, $x_{\text{rt}}(\ell) \sim \frac{1}{\ell}$ for $Z^{10^{-9}} < \ell < \Omega$. In $(x_{\text{left}}(\ell), x_{\text{rt}}(\ell))$ we have $0 < -V_\ell(r) = -V(r) - \frac{\ell(\ell+1)}{r^2} < -V(r) < C\min\{\frac{Z}{r}, r^{-4}\}$, and therefore we have $\big(-V_\ell(r)\big)_+^{-1/2} \ge c\big[\min\{\frac{Z}{r}, r^{-4}\}\big]^{-1/2}\chi_{(x_{\text{left}}(\ell),x_{\text{rt}}(\ell))}(r)$ for all r. For ℓ small compared to $\Omega \sim Z^{1/3}$, we have also $x_{\text{left}}(\ell) << Z^{-1/3} << x_{\text{rt}}(\ell)$, and thus

$$n_\ell = \int_0^\infty \big(-V_\ell(r)\big)_+^{-1/2}dr \ge c\int_{x_{\text{left}}(\ell)}^{x_{\text{rt}}(\ell)} \big[\min\{\frac{Z}{r}, r^{-4}\}\big]^{-1/2}dr$$
$$= c\int_{x_{\text{left}}(\ell)}^{Z^{-1/3}} \big(\frac{r}{Z}\big)^{1/2}dr + c\int_{Z^{-1/3}}^{x_{\text{rt}}(\ell)} r^2dr \sim \ell^{-3}\ .$$

This lower bound implies that

$$\Big|\sum_{Z^{10^{-9}}<\ell\le Z^{\frac{8}{25}+10\varepsilon}} \frac{2\ell+1}{n_\ell}\tilde{\chi}(\phi_\ell)\Big| \le C \sum_{Z^{10^{-9}}<\ell\le Z^{\frac{8}{25}+10\varepsilon}} \ell^4 \le C'(Z^{\frac{8}{25}+10\varepsilon})^5$$
$$= C'Z^{\frac{8}{5}+50\varepsilon} << Z^{\frac{8}{5}+2\cdot10^{-9}}\ .$$

for ε smaller than $2\cdot 10^{-11}$. Consequently, the sum over $Z^{10^{-9}} < \ell < \Omega$ in (195) may be replaced by a sum over $Z^{\frac{8}{25}+10\varepsilon} < \ell < \Omega$. We record this result in the following statement.

Main Lemma on Eigenvalue Sums. *Suppose $V(r)$ is defined on $(0,\infty)$ and satisfies*

(A) $\left|\left(\frac{d}{dr}\right)^{\alpha} V(r)\right| \le C_\alpha \min\{\frac{Z}{r}, r^{-4}\} \cdot r^{-\alpha}$ *for all* $r \in (0,\infty), \alpha \ge 0$

(B) $\left|\left(\frac{d}{dr}\right)^{\alpha} \{V(r) - V_Z^{TF}(r)\}\right| \le c_0 \min\{\frac{Z}{r}, r^{-4}\} \cdot r^{-\alpha}$ *for all* $r \in (0,\infty)$ *and for* $0 \le \alpha \le 2$, *with* c_0 *a small, positive constant depending on the* C_α *in (A).*

(C) $V(r) = E_0 - \frac{Z}{r}$ *for* $0 < r < Z^{-\frac{3}{5}+2\varepsilon}$, *with* $cZ^{4/3} < E_0 < CZ^{4/3}$ *and* $\varepsilon < 10^{-12}$.

We write $V(x)$ for the radial function $V(|x|)$ on $\mathbb{R}^3$. Then the sum of the negative eigenvalues of $-\Delta + V(x)$ is given by

$$-\frac{1}{15\pi^2}\int_{\mathbb{R}^3}\left(-V(x)\right)^{5/2}dx + \frac{Z^2}{8} + \frac{1}{48\pi^2}\int_{\mathbb{R}^3}\left(\Delta V(x)\right)\cdot\left(-V(x)\right)^{1/2}dx$$
$$+\pi \sum_{Z^{\frac{8}{25}+10\varepsilon}<\ell<\Omega} \frac{(2\ell+1)}{n_\ell}\tilde{\chi}(\phi_\ell) + \text{ Error },$$

with $|\text{Error}| < C' Z^{\frac{8}{5}+2\cdot 10^{-9}}$ *and* n_ℓ, ϕ_ℓ, Ω *defined by*

$$\Omega = \text{ positive root of } \Omega(\Omega+1) = \max_{r>0}\left(-r^2 V(r)\right)$$
$$n_\ell = \int_0^\infty \left(-V(r) - \frac{\ell(\ell+1)}{r^2}\right)_+^{-1/2} dr$$
$$\phi_\ell = \frac{1}{\pi}\int_0^\infty \left(-V(r) - \frac{\ell(\ell+1)}{r^2}\right)_+^{1/2} dr - \frac{1}{2}.$$

The constant C' depends only on c, C, C_α, ε in (A), (B), (C).

Proof. We saw that the sum in (195) could be restricted to a smaller range of ℓ as in the statement of the Main Lemma. Since $\Delta V(x) = \left(V'' + \frac{2}{r}V'\right)\big|_{r=|x|}$ and dvol $= 4\pi r^2 dr$, our present conclusion is equivalent to (195), (196). ∎

Perturbation of Eigenvalue Sums

In the previous section, we computed the sum of the negative eigenvalues of $-\Delta + V(|x|)$ under the restrictive assumption that $V(r) = E_0 - \frac{Z}{r}$ exactly when r is small. In this section, we use simple perturbation theory, together with our three-dimensional density results, to remove the restrictive assumption. We take $V(r)$ to satisfy the following conditions.

(1) $$\left|\left(\frac{d}{dr}\right)^\alpha V(r)\right| \leq C_\alpha \min\left\{\frac{Z}{r}, r^{-4}\right\} \cdot r^{-\alpha} \quad \text{for } r \in (0,\infty), \alpha \geq 0$$

(2)
$$\left|\left(\frac{d}{dr}\right)^\alpha \left\{V(r) - V_Z^{TF}(r)\right\}\right| \leq c_0 \cdot \min\left\{\frac{Z}{r}, r^{-4}\right\} \cdot r^{-\alpha} \text{ for } r \in (0,\infty)\ , 0 \leq \alpha \leq 2\ ;$$

with c_0 a small, positive constant depending on C_α .

(3) $$\left|\left(\frac{d}{dr}\right)^\alpha \left\{V(r) - \left[E_0 - \frac{Z}{r}\right]\right\}\right| \leq C_\alpha Z^{\frac{3}{2}} r^{\frac{1}{2}} \cdot r^{-\alpha}$$

for $r \in (0, 2Z^{-\frac{3}{5}+2\varepsilon}), \alpha \geq 0$. Here $0 < \varepsilon < 10^{-12}$, and $cZ^{4/3} < E_0 < CZ^{4/3}$.

Note that $V(r) = V_Z^{TF}(r)$ satisfies (1), (2), (3).

We shall prove that the conclusion of the Main Lemma of the previous section holds under the weakened hypotheses (1), (2), (3). We start by modifying $V(r)$ to satisfy the hypotheses of the Main Lemma.

Take $\theta(r) = 1$ for $r \leq Z^{-\frac{3}{5}+2\varepsilon}$, $\theta(r) = 0$ for $r \geq 2 \cdot Z^{-\frac{3}{5}+2\varepsilon}$, with

$$\left|\left(\frac{d}{dr}\right)^\alpha \theta(r)\right| \leq C_\alpha r^{-\alpha} \quad \text{for all } r\ .$$

Then set $V_1(r) = V(r) + \theta(r) \cdot \left[E_0 - \frac{Z}{r} - V(r)\right]$. For $0 < r < Z^{-\frac{3}{5}+2\varepsilon}$, we have $V_1(r) = E_0 - \frac{Z}{r}$, which is hypothesis (C) of the Main Lemma.

¿From (3) and the properties of θ, we get

(4) $$\left|\left(\frac{d}{dr}\right)^\alpha \left\{\theta(r) \cdot \left[E_0 - \frac{Z}{r} - V(r)\right]\right\}\right| \leq C'_\alpha Z^{\frac{3}{2}} r^{\frac{1}{2}-\alpha} = C'_\alpha \frac{Z}{r} \cdot r^{-\alpha} \cdot (Z^{1/2} r^{3/2})$$
$$\leq C''_\alpha \frac{Z}{r} \cdot r^{-\alpha} \cdot (Z^{1/2} \cdot Z^{-\frac{9}{10}+3\varepsilon})$$
$$= C''_\alpha \frac{Z}{r} \cdot r^{-\alpha} \cdot Z^{-\frac{2}{5}+3\varepsilon} \text{ in supp } \theta\ .$$

Therefore,

$$\Big|\big(\frac{d}{dr}\big)^{\alpha}V_1(r)\Big| \le C_\alpha \min\{\frac{Z}{r}, r^{-4}\}r^{-\alpha} + C''_\alpha Z^{-\frac{2}{5}+3\varepsilon}\min\{\frac{Z}{r}, r^{-4}\}r^{-\alpha}$$

by (1); and for $0 \le \alpha \le 2$ we have

$$\Big|\big(\frac{d}{dr}\big)^{\alpha}\{V_1(r) - V_Z^{TF}(r)\}\Big| \le \Big|\big(\frac{d}{dr}\big)^{\alpha}\{V(r) - V_Z^{TF}(r)\}\Big| + C''Z^{-\frac{2}{5}+3\varepsilon}\min\{\frac{Z}{r}, r^{-4}\}r^{-\alpha} \le 2c_0\min\{\frac{Z}{r}, r^{-4}\}r^{-\alpha} \text{ by (2)} .$$

These estimates imply hypotheses (A) and (B) for the potential V_1. Thus, we may apply the Main Lemma of the previous section to V_1, obtaining

(5)
$$\mathrm{sneg}(-\Delta+V_1) = -\frac{1}{15\pi^2}\int_{\mathbb{R}^3}\big(-V_1(x)\big)^{5/2}dx + \frac{Z^2}{8} + \frac{1}{48\pi^2}\int_{\mathbb{R}^3}(\Delta V_1(x))\cdot\big(-V_1(x)\big)^{1/2}dx + \pi\sum_{Z^{\frac{8}{25}+10\varepsilon}<\ell<\Omega}\frac{(2\ell+1)}{n_\ell}\tilde{\chi}(\phi_\ell) + \text{ Error}_1 ,$$

with

(6) $$|\mathrm{Error}_1| \le C'Z^{\frac{8}{5}+2\cdot 10^{-9}}$$

(7) $$\Omega = \text{ pos. root of } \Omega(\Omega+1) = \max_{r>0}\big(-r^2V_1(r)\big)$$

(8) $$n_\ell = \int_0^\infty\Big(-V_1(r) - \frac{\ell(\ell+1)}{r^2}\Big)_+^{-1/2}dr \quad (Z^{\frac{8}{25}+10\varepsilon} < \ell < \Omega)$$

(9) $$\phi_\ell = \frac{1}{\pi}\int_0^\infty\Big(-V_1(r) - \frac{\ell(\ell+1)}{r^2}\Big)_+^{1/2}dr - \frac{1}{2} \quad (Z^{\frac{8}{25}+10\varepsilon} < \ell < \Omega) .$$

Here we write V, V_1 both for functions of one variable, and for the corresponding radial functions on $\mathbb{R}^3$.

In (7), (8), (9), we can replace $V_1(r)$ by $V(r)$ without changing the values of Ω, n_ℓ, ϕ_ℓ. In fact, (2) shows that $-r^2V(r)$ is an increasing function on $(0, 2Z^{-\frac{3}{5}+2\varepsilon})$.

Similarly, $-r^2V_1(r)$ is increasing on $(0, 2Z^{-\frac{3}{5}+3\varepsilon})$, by virtue of hypotheses (A) and (B) of the Main Lemma, which we know to be valid for V_1. Hence, the maxima of $-r^2V(r)$ and $-r^2V_1(r)$ are both attained in $(2Z^{-\frac{3}{5}+2\varepsilon}, \infty)$, where $V \equiv V_1$.

Consequently, changing $V_1(r)$ to $V(r)$ in (7) leaves the value of Ω unchanged. To see that (8), (9) are also unchanged, suppose $\ell > Z^{\frac{8}{25}+10\varepsilon}$. Then for $0 < r < 2Z^{-\frac{3}{5}+2\varepsilon}$ we have

$$|V(r)|, |V_1(r)| \le C \min\{\frac{Z}{r}, r^{-4}\} = C\frac{Z}{r} = \frac{\ell(\ell+1)}{r^2} \cdot \frac{CZr}{\ell(\ell+1)}$$
$$\le \frac{\ell(\ell+1)}{r^2} \cdot \left[\frac{C'Z \cdot Z^{-\frac{3}{5}+2\varepsilon}}{Z^{\frac{16}{25}+20\varepsilon}}\right] < \frac{\ell(\ell+1)}{r^2} \, .$$

Hence, $-V(r) - \frac{\ell(\ell+1)}{r^2}$ and $-V_1(r) - \frac{\ell(\ell+1)}{r^2}$ are both negative when $\ell > Z^{\frac{8}{25}+10\varepsilon}$ and $r < 2Z^{-\frac{3}{5}+2\varepsilon}$. This implies

$$\int_0^\infty \left(-V_1(r) - \frac{\ell(\ell+1)}{r^2}\right)_+^{-1/2} dr = \int_{2Z^{-\frac{3}{5}+2\varepsilon}}^\infty \left(-V_1(r) - \frac{\ell(\ell+1)}{r^2}\right)_+^{-1/2} dr$$
$$= \int_{2Z^{-\frac{3}{5}+2\varepsilon}}^\infty \left(-V(r) - \frac{\ell(\ell+1)}{r^2}\right)_+^{-1/2} dr = \int_0^\infty \left(-V(r) - \frac{\ell(\ell+1)}{r^2}\right)_+^{-1/2} dr$$

for $\ell > Z^{\frac{8}{25}+10\varepsilon}$, so (8) is unaffected when we replace $V_1(r)$ by $V(r)$. Similarly for (9). Thus,

(10)
$$\text{sneg}(-\Delta+V_1) = -\frac{1}{15\pi^2}\int_{\mathbb{R}^3}\left(-V_1(x)\right)^{5/2}dx + \frac{Z^2}{8} + \frac{1}{48\pi^2}\int_{\mathbb{R}^3}\left(\Delta V_1(x)\right)\cdot\left(-V_1(x)\right)^{1/2}dx$$
$$+ \pi \sum_{Z^{\frac{8}{25}+10\varepsilon}<\ell<\Omega} \frac{(2\ell+1)}{n_\ell}\tilde{\chi}(\phi_\ell) + \text{ Error}_1 \; , \quad \text{with}$$

(11)
$$\Omega = \text{ pos. root of } \Omega(\Omega+1) = \max_{r>0}\left(-r^2V(r)\right)$$

(12)
$$n_\ell = \int_0^\infty \left(-V(r) - \frac{\ell(\ell+1)}{r^2}\right)_+^{-1/2} dr$$

(13)
$$\phi_\ell = \frac{1}{\pi}\int_0^\infty \left(-V(r) - \frac{\ell(\ell+1)}{r^2}\right)_+^{1/2} dr - \frac{1}{2}$$

$$|\text{Error}_1| \leq C' Z^{\frac{8}{5}+2\cdot 10^{-9}} . \tag{14}$$

We want to compare $\text{sneg}(-\Delta+V_1)$ with $\text{sneg}(-\Delta+V)$. Let $E_1, \ldots, E_N$ be the non-positive eigenvalues of $-\Delta+V_1$, and let $\varphi_1(x)\ldots\varphi_N(x)$ be the corresponding normalized eigenfunctions. We introduce the N-particle wave function

$$\psi(x_1\ldots x_N) = \frac{1}{\sqrt{N!}}\sum_\sigma (\text{sgn }\sigma)\varphi_{\sigma 1}(x_1)\ldots\varphi_{\sigma N}(x_N) , \tag{15}$$

where σ denotes a permutation of $\{1\ldots N\}$. Thus, ψ is antisymmetric and has norm 1. Moreover,

$$\begin{aligned} \text{sneg}(-\Delta+V_1) &= E_1+\ldots+E_N = \langle\sum_{k=1}^N\big(-\Delta_{x_k}+V_1(x_k)\big)\psi,\psi\rangle \\ &= \langle\sum_{k=1}^N\big(-\Delta_{x_k}+V(x_k)\big)\psi,\psi\rangle + \langle\sum_{k=1}^N\big(V_1(x_k)-V(x_k)\big)\psi,\psi\rangle \\ &\geq \ \text{sneg}(-\Delta+V) + \langle\sum_{k=1}^N\big(V_1(x_k)-V(x_k)\big)\psi,\psi\rangle , \end{aligned} \tag{16}$$

as follows by expanding $\psi(x_1\ldots x_N)$ in terms of the eigenfunctions of $-\Delta+V(x)$. For the wave function (15), we have

$$\langle\sum_{k=1}^N\big(V_1(x_k)-V(x_k)\big)\psi,\psi\rangle = \int_{\mathbb{R}^3}\rho_1(x)\big(V_1(x)-V(x)\big)dx , \tag{17}$$

where

$$\rho_1(x) = \sum_{k=1}^N |\varphi_k(x)|^2 = \text{ density associated to } -\Delta+V_1 . \tag{18}$$

Putting (17) into (16), we get the inequality

$$\text{sneg}(-\Delta+V_1) \geq \ \text{sneg}(-\Delta+V) + \int_{\mathbb{R}^3}\rho_1(x)\big(V_1(x)-V(x)\big)dx . \tag{19}$$

Similarly, reversing the roles of V_1 and V in the last paragraph, we find that

$$\text{sneg}(-\Delta+V) \geq \ \text{sneg}(-\Delta+V_1) + \int_{\mathbb{R}^3}\rho(x)\cdot\big(V(x)-V_1(x)\big)dx , \tag{20}$$

where $\rho(x)$ is the density associated to $-\Delta + V$.

In (19), (20) we want to replace ρ_1 and ρ by their semiclassical approximations. Hence we rewrite these inequalities in the form

$$\text{(21)}\quad \operatorname{sneg}(-\Delta + V_1) \geq \operatorname{sneg}(-\Delta + V) + \frac{1}{6\pi^2}\int_{\mathbb{R}^3} \big(-V_1(x)\big)^{3/2}\big(V_1(x) - V(x)\big)dx + \int_{\mathbb{R}^3}\Big[\rho_1(x) - \frac{1}{6\pi^2}\big(-V_1(x)\big)^{3/2}\Big]\big(V_1(x) - V(x)\big)dx$$

$$\text{(22)}\quad \operatorname{sneg}(-\Delta + V) \geq \operatorname{sneg}(-\Delta + V_1) + \frac{1}{6\pi^2}\int_{\mathbb{R}^3} \big(-V(x)\big)^{3/2}\big(V(x) - V_1(x)\big)dx + \int_{\mathbb{R}^3}\Big[\rho(x) - \frac{1}{6\pi^2}\big(-V(x)\big)^{3/2}\Big]\big(V(x) - V_1(x)\big)dx\ .$$

We can control the integrals at the far right in (21), (22) by using Theorem 1 in the section on the WKB Density Theorems for Approximate TF Potentials. Since

$$V_1(x) - V(x) = \theta(r)\cdot\Big[E_0 - \frac{Z}{r} - V(r)\Big]\ (r = |x|)\ ,$$

estimate (3) and the properties of $\theta(r)$ allow us to write

$$\text{(23)}\qquad V_1(x) - V(x) = \sum_{k=1}^{\infty}(Z^{3/2}\delta_k^{1/2})U_k(x)\ ,$$

where: $U_k(x)$ is a radial function supported in $\delta_k < |x| < 2\delta_k$, $|U_k(x)| \leq C$, $|\nabla U_k(x)| \leq C\delta_k^{-1}$, $\delta_{k+1} \leq (1-c)\delta_k$, $\delta_1 \sim Z^{-\frac{3}{5}+2\varepsilon}$.

From (23) and the Lebesgue dominated convergence theorem, we get

$$\text{(24)}\quad \int_{\mathbb{R}^3}\Big[\rho_1(x) - \frac{\big(-V_1(x)\big)^{3/2}}{6\pi^2}\Big]\cdot\big(V_1(x) - V(x)\big)dx = \sum_{k=1}^{\infty} Z^{3/2}\delta_k^{1/2}\int_{\mathbb{R}^3}\Big[\rho_1(x) - \frac{\big(-V_1(x)\big)^{3/2}}{6\pi^2}\Big]U_k(x)dx\ .$$

Theorem 1 in the section on the Density for Approximate TF Potentials shows that

$$\Big|\int_{\mathbb{R}^3}\Big[\rho_1(x) - \frac{\big(-V_1(x)\big)^{3/2}}{6\pi^2}\Big]U_k(x)dx\Big| \leq C'\big(Z\delta_k + Z^{\frac{1}{3}+2\cdot 10^{-9}}\big)\ .$$

This and (24) imply

$$(25)\quad \left|\int_{\mathbb{R}^3}\left[\rho_1(x)-\frac{1}{6\pi^2}\big(-V_1(x)\big)^{3/2}\right]\cdot\big(V_1(x)-V(x)\big)\,dx\right|$$
$$\leq C\sum_{k=1}^{\infty} Z^{3/2}\delta_k^{1/2}\big(Z\delta_k+Z^{\frac13+2\cdot10^{-9}}\big)$$
$$=C\sum_{k=1}^{\infty} Z^{5/2}\delta_k^{3/2}+C\sum_{k=1}^{\infty} Z^{\frac{11}{6}+2\cdot10^{-9}}\delta_k^{1/2}$$
$$\sim Z^{5/2}\delta_1^{3/2}+Z^{\frac{11}{6}+2\cdot10^{-9}}\delta_1^{1/2}$$
$$\sim Z^{5/2}\big(Z^{-\frac35+2\varepsilon}\big)^{\frac32}+Z^{\frac{11}{6}+2\cdot10^{-9}}\big(Z^{-\frac35+2\varepsilon}\big)^{1/2}\sim Z^{\frac85+3\varepsilon}\ .$$

Similarly,

$$(26)\qquad \left|\int_{\mathbb{R}^3}\left[\rho(x)-\frac{1}{6\pi^2}\big(-V(x)\big)^{3/2}\right]\cdot\big(V_1(x)-V(x)\big)\,dx\right|\leq CZ^{\frac85+3\varepsilon}\ .$$

Putting (25), (26) into (21), (22), we find that

$$(27)\quad \mathrm{sneg}(-\Delta+V_1)\geq\ \mathrm{sneg}(-\Delta+V)+\frac{1}{6\pi^2}\int_{\mathbb{R}^3}\big(-V_1(x)\big)^{3/2}\big(V_1(x)-V(x)\big)\,dx$$
$$-\,CZ^{\frac85+3\varepsilon}$$

and

$$(28)\quad \mathrm{sneg}(-\Delta+V)\geq\ \mathrm{sneg}(-\Delta+V_1)+\frac{1}{6\pi^2}\int_{\mathbb{R}^3}\big(-V(x)\big)^{3/2}\big(V(x)-V_1(x)\big)\,dx$$
$$-\,CZ^{\frac85+3\varepsilon}\ .$$

In the integral in (27) we want to replace $\big(-V_1(x)\big)^{3/2}$ by $\big(-V(x)\big)^{3/2}$.

Recall that $V_1(r)-V(r)$ is supported in $\big[0,2Z^{\frac35+2\varepsilon}\big]$ and is dominated by $Z^{3/2}r^{1/2}$; while $-V(r)\sim Zr^{-1}$ in that interval. Hence we can write

$$(29)\qquad V_1(r)=\big(1+f_1(r)\big)V(r)\ ,\qquad f_1(r)=\big(V(r)-V_1(r)\big)\big(-V(r)\big)^{-1}$$

with $f_1(r)$ supported in $\big[0,2Z^{-\frac35+2\varepsilon}\big]$, and with

$$(30)\qquad |f_1(r)|\leq CZ^{1/2}r^{3/2}\ .$$

Therefore, for any exponent p we have

$$\begin{aligned}
\big(-V_1(r)\big)^p &= \big(1 + pf_1(r) + O(|f_1(r)|^2)\big) \cdot \big(-V(r)\big)^p \\
&= \big(1 + pf_1(r)\big) \cdot \big(-V(r)\big)^p + O(Zr^3 \cdot Z^p r^{-p}) \\
&= \big(-V(r)\big)^p + p\big(V(r) - V_1(r)\big) \cdot \big(-V(r)\big)^{p-1} + O(Z^{p+1} r^{3-p}) \ . \qquad (31)
\end{aligned}$$

In particular,

$$\begin{aligned}
\big|\big(-V_1(r)\big)^{3/2} - \big(-V(r)\big)^{3/2}\big| &\le C|V(r) - V_1(r)| \cdot \big(-V(r)\big)^{1/2} + CZ^{\frac{5}{2}} r^{3/2} \\
&\le CZ^{3/2} r^{1/2} \cdot (Zr^{-1})^{1/2} + CZ^{5/2} r^{3/2} \\
&\le CZ^2 \quad \text{for } r \in [0, 2Z^{-\frac{3}{5}+2\varepsilon}] \ ,
\end{aligned}$$

so

$$\begin{aligned}
&\Big| \int_{\mathbb{R}^3} \big(-V(x)\big)^{3/2} \big(V_1(x) - V(x)\big) dx - \int_{\mathbb{R}^3} \big(-V_1(x)\big)^{3/2} \big(V_1(x) - V(x)\big) dx \Big| \\
&\qquad \le \int_{|x| < 2Z^{-\frac{3}{5}+2\varepsilon}} CZ^2 |V_1(x) - V(x)| \ \mathrm{dvol}(x) \\
&\qquad \le \int_0^{2Z^{-\frac{3}{5}+2\varepsilon}} CZ^2 \cdot (CZ^{3/2} r^{1/2}) \cdot r^2 dr \sim Z^{\frac{7}{2}} \cdot (2Z^{-\frac{3}{5}+2\varepsilon})^{\frac{7}{2}} \ \sim Z^{\frac{7}{5}+7\varepsilon} \ .
\end{aligned}$$

Combining this with (27), we get

$$\begin{aligned}
\mathrm{sneg}(-\Delta + V_1) \ge \ \mathrm{sneg}(-\Delta + V) + \frac{1}{6\pi^2} \int_{\mathbb{R}^3} \big(-V(x)\big)^{3/2} \big(V_1(x) - V(x)\big) dx \\
- CZ^{\frac{8}{5}+3\varepsilon} \ ,
\end{aligned}$$

which together with (28) implies

(32)

$$\mathrm{sneg}(-\Delta + V) = \ \mathrm{sneg}(-\Delta + V_1) + \frac{1}{6\pi^2} \int_{\mathbb{R}^3} \big(-V(x)\big)^{3/2} \big(V(x) - V_1(x)\big) dx + \ \mathrm{Error}_2$$

with $|\mathrm{Error}_2| \le CZ^{\frac{8}{5}+3\varepsilon}$.

Putting (10) into the right-hand side of (32), we obtain

(33)

$$\mathrm{sneg}(-\Delta+V) = \Big\{-\frac{1}{15\pi^2}\int_{\mathbb{R}^3}\big(-V_1(x)\big)^{5/2}dx+\frac{1}{6\pi^2}\int_{\mathbb{R}^3}\big(-V(x)\big)^{3/2}\big(V(x)-V_1(x)\big)dx\Big\} + \frac{Z^2}{8} + \frac{1}{48\pi^2}\int_{\mathbb{R}^3}\big(\Delta V_1(x)\big)\cdot\big(-V_1(x)\big)^{1/2}dx + \pi\sum_{Z^{\frac{8}{25}+10\varepsilon}<\ell<\Omega}\frac{(2\ell+1)}{n_\ell}\tilde{\chi}(\phi_\ell) + \text{ Error}_3\ ,$$

with

(34) $$|\text{Error}_3| \leq CZ^{\frac{8}{5}+2\cdot 10^{-9}}\ .$$

¿From (31) with $p=\frac{5}{2}$, we get

$$\Big\{-\frac{1}{15\pi^2}\int_{\mathbb{R}^3}\big(-V_1(x)\big)^{5/2}dx+\frac{1}{6\pi^2}\int_{\mathbb{R}^3}\big(-V(x)\big)^{3/2}\big(V(x)-V_1(x)\big)dx\Big\} = -\frac{1}{15\pi^2}\int_{\mathbb{R}^3}\Big[\big(-V(x)\big)^{5/2}+\frac{5}{2}\big(V(x)-V_1(x)\big)\cdot\big(-V(x)\big)^{3/2}+g(x)\Big]dx + \frac{1}{6\pi^2}\int_{\mathbb{R}^3}\big(-V(x)\big)^{3/2}\big(V(x)-V_1(x)\big)dx$$

with

$$|g(x)| \leq CZ^{7/2}|x|^{1/2}\chi_{|x|<2Z^{-\frac{3}{5}+2\varepsilon}}\ .$$

That is,

$$\Big\{-\frac{1}{15\pi^2}\int_{\mathbb{R}^3}\big(-V_1(x)\big)^{5/2}dx+\frac{1}{6\pi^2}\int_{\mathbb{R}^3}\big(-V(x)\big)^{3/2}\big(V(x)-V_1(x)\big)dx\Big\} = -\frac{1}{15\pi^2}\int_{\mathbb{R}^3}\big(-V(x)\big)^{5/2}dx-\frac{1}{15\pi^2}\int_{\mathbb{R}^3}g(x)dx\ ,$$

with the last term on the right dominated by

$$\int_0^{2Z^{-\frac{3}{5}+2\varepsilon}} Z^{\frac{7}{2}}r^{1/2}\cdot r^2dr \sim Z^{\frac{7}{2}}(2Z^{-\frac{3}{5}+2\varepsilon})^{\frac{7}{2}} \sim Z^{\frac{7}{5}+7\varepsilon}\ .$$

So the expression in curly brackets is (33) is equal to $-\frac{1}{15\pi^2}\int_{\mathbb{R}^3}\big(-V(x)\big)^{5/2}dx + O(Z^{\frac{7}{5}+7\varepsilon})$. Consequently, (33) and (34) may be rewritten as

(35)

$$\mathrm{sneg}(-\Delta+V) = -\frac{1}{15\pi^2}\int_{\mathbb{R}^3}\big(-V(x)\big)^{5/2}dx+\frac{Z^2}{8}+\frac{1}{48\pi^2}\int_{\mathbb{R}^3}\big(\Delta V_1(x)\big)\big(-V_1(x)\big)^{1/2}dx + \pi\sum_{Z^{\frac{8}{25}+10\varepsilon}<\ell<\Omega}\frac{(2\ell+1)}{n_\ell}\tilde{\chi}(\phi_\ell) + \text{ Error}_4$$

with

$$|\mathrm{Error}_4| \le CZ^{\frac{8}{5}+2\cdot 10^{-9}} . \tag{36}$$

We want to replace V_1 by V in the second integral in (35). We have

$$\Big| \int_{\mathbb{R}^3} (\Delta V_1)\big(-V_1(x)\big)^{1/2} dx - \int_{\mathbb{R}^3} (\Delta V)\big(-V(x)\big)^{1/2} dx \Big| \tag{37}$$
$$\le \int_{\mathbb{R}^3} |\Delta V - \Delta V_1| \cdot \big(-V_1(x)\big)^{1/2} dx + \int_{\mathbb{R}^3} |\Delta V| \cdot |(-V_1)^{1/2} - (-V)^{1/2}| dx .$$

From (3) and the properties of θ, we have

$$\big|\Delta(V - V_1)\big| = \Big|\Big(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\Big)\big\{\theta(r)\big[E_0 - \frac{Z}{r} - V(r)\big]\big\}\Big| \le CZ^{3/2} r^{-3/2} , \ r = |x| .$$

Also,

$$\big(-V_1(x)\big)^{1/2} \sim Z^{1/2} r^{-1/2} \quad \text{in} \quad \mathrm{supp}\,(V - V_1) \subset \big\{|x| < 2Z^{-\frac{3}{5}+2\varepsilon}\big\} .$$

Hence

(38)

$$\int_{\mathbb{R}^3} |\Delta V - \Delta V_1| \cdot \big(-V(x)\big)^{1/2} dx \le C \int_0^{2Z^{-\frac{3}{5}+2\varepsilon}} (Z^{3/2} r^{-3/2}) \cdot (Z^{1/2} r^{-1/2}) \cdot r^2 dr$$
$$\sim Z^2 \cdot 2Z^{-\frac{3}{5}+2\varepsilon} \sim Z^{\frac{7}{5}+2\varepsilon} .$$

On the other hand, (1) yields $|\Delta V| \le CZr^{-3}$ in $\mathrm{supp}\,(V_1 - V)$; and (31) shows that

$$\big|\big(-V(x)\big)^{1/2} - \big(-V_1(x)\big)^{1/2}\big| \le C|V(x) - V_1(x)| \cdot \big(-V(x)\big)^{-1/2} + CZ^{\frac{3}{2}} r^{\frac{5}{2}}$$
$$\le C(Z^{3/2} r^{1/2}) \cdot (Zr^{-1})^{-1/2} + CZ^{\frac{3}{2}} r^{5/2}$$
$$= CZr + CZ^{\frac{3}{2}} r^{5/2} = CZr(1 + Z^{\frac{1}{2}} r^{\frac{3}{2}})$$
$$\le C'Zr \qquad \text{in} \quad \mathrm{supp}\,(V - V_1) .$$

Therefore,

$$\int_{\mathbb{R}^3} |\Delta V(x)| \cdot \big|\big(-V(x)\big)^{1/2} - \big(-V_1(x)\big)^{1/2}\big| dx$$
$$\le C \int_0^{2Z^{-\frac{3}{5}+2\varepsilon}} (Zr^{-3}) \cdot (Zr) \cdot r^2 dr \sim Z^2 \cdot (2Z^{-\frac{3}{5}+2\varepsilon}) \sim Z^{\frac{7}{5}+2\varepsilon} .$$

Putting this and (38) into (37), we see that

$$\Big| \int_{\mathbb{R}^3} (+\Delta V_1)\cdot(-V_1)^{1/2}dx - \int_{\mathbb{R}^3} (+\Delta V)\cdot(-V)^{1/2}dx \Big| \le CZ^{\frac{7}{5}+2\varepsilon} .$$

Hence, equations (35), (36) may be rewritten in the form

(39)

$$\begin{aligned} \mathrm{sneg}(-\Delta+V) = -\frac{1}{15\pi^2}\int_{\mathbb{R}^3}\big(-V(x)\big)^{5/2}dx + \frac{Z^2}{8} + \frac{1}{48\pi^2}\int_{\mathbb{R}^3}\big(\Delta V(x)\big)\cdot\big(-V(x)\big)^{1/2}dx \\ + \pi \sum_{Z^{\frac{8}{25}+10\varepsilon}<\ell<\Omega} \frac{(2\ell+1)}{n_\ell}\tilde{\chi}(\phi_\ell) + \ \mathrm{Error}_5 \ , \end{aligned}$$

with

(40) $$|\mathrm{Error}_5| \le CZ^{\frac{8}{5}+2\cdot 10^{-9}} .$$

We record equations (11), (12), (13), (39), (40) in the Theorem of the next section.

The WKB Eigenvalue Sum Theorem for Approximate TF Potentials

Suppose $V(r)$ is defined on $(0,\infty)$, and satisfies the following conditions.

(1) $$\Big|\big(\frac{d}{dr}\big)^{\alpha} V(r)\Big| \le C_\alpha \min\big\{\frac{Z}{r}, r^{-4}\big\}\cdot r^{-\alpha} \quad \text{for all } r\in(0,\infty)\ , \alpha\ge 0\ .$$

(2) $$\Big|\big(\frac{d}{dr}\big)^{\alpha}\big\{V(r)-V_Z^{TF}(r)\big\}\Big| \le c_0 \min\big\{\frac{Z}{r}, r^{-4}\big\}\cdot r^{-\alpha}$$

for $0\le\alpha\le 2$ and $r\in(0,\infty)$, with $c_0>0$ determined by the C_α in (1) .

(3) $$\Big|\big(\frac{d}{dr}\big)^{\alpha}\big\{E_0-\frac{Z}{r}-V(r)\big\}\Big| \le C_\alpha Z^{\frac{3}{2}}\, r^{\frac{1}{2}-\alpha}$$

for $\alpha\ge 0$ and $r\in(0,2Z^{-\frac{3}{5}+2\varepsilon})$, with $cZ^{4/3}<E_0<CZ^{4/3}$ and $0<\varepsilon<10^{-12}$.

Write $V(x)$ for the radial function $V(|x|)$ on $\mathbb{R}^3$, and set $H=-\Delta+V(x)$ on $\mathbb{R}^3$. Set $\Omega=$ positive root of $\Omega(\Omega+1)=\max\limits_{r>0}\big(-r^2V(r)\big)$, and define

$$n_\ell = \int_0^\infty \Big(-V(r)-\frac{\ell(\ell+1)}{r^2}\Big)_+^{-1/2} dr\ ,$$

$$\phi_\ell = \frac{1}{\pi}\int_0^\infty \Big(-V(r)-\frac{\ell(\ell+1)}{r^2}\Big)_+^{1/2} dr - \frac{1}{2} \qquad \text{for } 1\le\ell<\Omega\ .$$

Then the sum of the negative eigenvalues of H is given by

$$\text{sneg}(H) = -\frac{1}{15\pi^2}\int_{\mathbb{R}^3}(-V)^{5/2}dx + \frac{Z^2}{8} + \frac{1}{48\pi^2}\int_{\mathbb{R}^3}(\Delta V)\cdot(-V)^{1/2}dx$$
$$+\pi \sum_{Z^{\frac{8}{25}+10\varepsilon}<\ell<\Omega} \frac{(2\ell+1)}{n_\ell}\tilde{\chi}(\phi_\ell) + \text{Error}\ ,$$

with

$$|\text{Error}| \le C' Z^{\frac{8}{5}+2\cdot 10^{-9}}\ .$$

The constant C' depends only on C_α, c, C, ε in (1), (2), (3).

Proof. The conclusion is contained in equations (11), (12), (13), (39), (40) in the preceding section. ■

Estimates for Number-Theoretic Sums

Let $V(r)$, Ω, n_ℓ, ϕ_ℓ be as in the WKB Eigenvalue Sum Theorem for Approximate TF Potentials. Thus, we assume:

$$\left|\left(\frac{d}{dr}\right)^\alpha V(r)\right| \le C_\alpha \min\left\{\frac{Z}{r}, r^{-4}\right\} \cdot r^{-\alpha} \quad \text{for } \alpha \ge 0 \;\; r > 0 \; ; \tag{1}$$

$$\left|\left(\frac{d}{dr}\right)^\alpha \left\{V(r) - V_Z^{TF}(r)\right\}\right| < c_0 \min\left\{\frac{Z}{r}, r^{-4}\right\} \cdot r^{-\alpha} \quad \text{for } \alpha \ge 0 \; , \;\; r > 0 \; , \tag{2}$$

with small $c_0 > 0$ determined by the C_α in (1);

$$\left|\left(\frac{d}{dr}\right)^\alpha \left\{E_0 - \frac{Z}{r} - V(r)\right\}\right| \le C_\alpha Z^{\frac{3}{2}} r^{\frac{1}{2}-\alpha} \quad \text{for } \alpha \ge 0 \; , \;\; 0 < r < 2Z^{-\frac{3}{5}+2\varepsilon} \; , \tag{3}$$

with $cZ^{4/3} < E_0 < CZ^{4/3}$ and $0 < \varepsilon < 10^{-12}$.

Recall that Ω, n_ℓ, ϕ_ℓ are defined as follows.

$$\Omega \text{ is the positive root of } \Omega(\Omega+1) = \max_{r>0}\left(-r^2 V(r)\right) \; ; \tag{4}$$

$$n_\ell = \int_0^\infty \left(-V(r) - \frac{\ell(\ell+1)}{r^2}\right)_+^{-1/2} \quad \text{for } 1 \le \ell < \Omega \; ; \tag{5}$$

$$\phi_\ell = \frac{1}{\pi}\int_0^\infty \left(-V(r) - \frac{\ell(\ell+1)}{r^2}\right)_+^{1/2} dr - \frac{1}{2} \quad \text{for } 1 \le \ell < \Omega \; . \tag{6}$$

To make full use of the WKB Density and Eigenvalue Sum Theorems for Approximate TF Potentials, we want to prove the following estimates for some $a > 0$.

$$\left|\sum_{\ell_1 \le \ell \le \ell_2} \frac{(2\ell+1)}{n_\ell} \chi_-(\phi_\ell)\right| \le C\Omega^{-2a} \sum_{\ell_1 \le \ell \le \ell_2} \frac{(2\ell+1)}{n_\ell} \tag{7}$$

$$\text{for } Z^{10^{-9}} \le \ell_1 < \ell_2 < \Omega \text{ with } \ell_2 - \ell_1 > \Omega^{1-10a} \; .$$

(8) There are at most $C\Omega^{1-6a}$ integers $\ell < \Omega$ for which

$$|\phi_\ell - \text{ nearest integer } | \le \ell^{-6/43} \; .$$

$$(9) \qquad \Big| \sum_{Z^{\frac{8}{25}+10\varepsilon} < \ell < \Omega} \frac{(2\ell+1)}{n_\ell} \tilde{\chi}(\phi_\ell) \Big| \le C\Omega^{-2a} Z^{5/3} \ .$$

These estimates are clearly related to the equidistribution of the ϕ_ℓ modulo 1. To prove them, we need an important extra assumption on the potential $V(r)$. With

$$(10) \qquad \Theta(t) = \int_0^\infty \left(-V(r) - \frac{t^2}{r^2}\right)_+^{1/2} dr \quad \text{for } 0 < t < (\max_{r>0}[-r^2 V(r)])^{1/2} \ ,$$

we assume

$$(11) \qquad \left|\frac{d^2}{dt^2}\Theta(t)\right| \ge cZ^{-1/3} \quad \text{for } Z^{10^{-9}} < t < (\max_{r>0}[-r^2 V(r)])^{1/2} \ .$$

In [FS6] we proved (11) for $V(r)$ close enough to the Thomas-Fermi potential $V_Z^{TF}(r)$ in a suitable metric. Here, we simply assume (11). Note that (11) fails for $V(r) = E_0 - \frac{Z}{r}$ and for $V(r) = \lambda^2(r^2 - \mu)$ (with, say, $\lambda \sim Z$, $\mu \sim Z^{-2/3}$), i.e. for the hydrogen atom and the harmonic oscillator. In these examples, $\frac{d^2}{dt^2}\Theta(t) = 0$, the ϕ_ℓ are not equidistributed modulo 1, the eigenvalues of $-\Delta + V$ are highly degenerate, and the desired semiclassical approximations to the density and eigenvalue sum are inaccurate. The failure of (11) is closely related to the periodicity of zero-energy orbits of a classical particle in the potential V.

All the number theory we need is contained in the following standard, elementary result. (Something more sophisticated would be needed to get the sharpest $a > 0$ in (7), (8), (9).)

Lemma 1. *Suppose $f(t)$, $\phi(t)$ are defined on an interval $[0, S]$ and satisfy there the estimates*

$$(12) \qquad |f(t)| \le C \ , \ |f'(t)| \le CR^{-1} \ , \ bR^{-1} \le \phi''(t) \le CR^{-1} \ , \textit{with } R \ge S \ge 10 \ .$$

Let $\chi(t)$ be a periodic function of period 1, having average zero and total variation on $[0, 1]$ given by

$$(13) \qquad \mathrm{Var}_{[0,1]}\chi \le C \ .$$

Then we have the estimate

$$\Big|\sum_{0\le k\le S} f(k)\chi(\phi(k))\Big| \le \frac{C'}{b}R^{2/3}\ell n R\ ,$$

with C' depending only on C in (12), (13).

Proof. Define a finite sequence $k_0, k_1, \ldots, k_{\nu_{\max}}$ inductively, as follows. We put $k_0 = 0$, and pick an integer N comparable to $R^{1/3}$. Suppose we have already defined $k_0, k_1, \ldots, k_\nu$. By the pigeon-hole principle, we can find integers p_ν, q_ν with

$$(14) \qquad 1 \le q_\nu \le N \quad \text{and} \quad |\phi'(k_\nu) - \frac{p_\nu}{q_\nu}| \le \frac{C}{q_\nu N}\ .$$

After dividing p_ν, q_ν by their greatest common divisor, we obtain (14) for p_ν and q_ν relatively prime. If $k_\nu + q_\nu \le S$, then define $k_{\nu+1} = k_\nu + q_\nu$.

If instead $k_\nu + q_\nu > S$, then define $\nu_{\max} = \nu$, so that the sequence $k_0, k_1, \ldots$ terminates at the given k_ν.

Note that the sequence must terminate eventually, since $k_{\nu+1} \ge k_\nu + 1$ for $0 \le \nu < \nu_{\max}$.

Using the integers $k_0 \ldots k_{\nu_{\max}}$, we break up $\sum_{0\le k\le S} f(k)\chi(\phi(k))$ into a sum of

$$X_\nu = \begin{cases} \sum_{k_\nu \le k < k_{\nu+1}} f(k)\chi(\phi(k)) & \text{for } 0 \le \nu < \nu_{\max} \\ \sum_{k_\nu \le k \le S} f(k)\chi(\phi(k)) & \text{for } \nu = \nu_{\max} \end{cases}\ .$$

Evidently,

$$(15) \qquad \sum_{0\le k\le S} f(k)\chi(\phi(k)) = \sum_{0\le\nu\le\nu_{\max}} X_\nu\ .$$

We estimate $X_{\nu_{\max}}$ trivially, by noting that $k_{\nu_{\max}} + N \ge k_{\nu_{\max}} + q_{\nu_{\max}} > S$. Hence the sum defining $X_{\nu_{\max}}$ has at most N terms. The terms are bounded, so

$$(16) \qquad |X_{\nu_{\max}}| \le CN\ .$$

For the other X_ν we will derive a much better estimate.

Fix $\nu < \nu_{\max}$, and set $\xi = \phi(k_\nu)$. Then for $k = k_\nu + m$ with $0 \le m < q_\nu$ we have

$$\phi(k) = \xi + \phi'(k_\nu) \cdot m + O(\frac{C}{R} m^2) \quad \text{by our bounds for } \phi'' \ .$$

Hence,

$$\phi(k) = \xi + \frac{p_\nu}{q_\nu} \cdot m + O\Big(\frac{m^2}{R} + |\phi'(k_\nu) - \frac{p_\nu}{q_\nu}| \cdot m\Big) \ .$$

The error is dominated by $\frac{N^2}{R} + \frac{C}{q_\nu N} \cdot q_\nu \le \frac{C}{N}$, since $0 \le m < q_\nu \le N$ and (14) holds. So

$$\phi(k) = \xi + \frac{p_\nu}{q_\nu} m + \tau_m \ , \quad \text{with } |\tau_m| \le \frac{C}{N} \ . \tag{17}$$

For $k = k_\nu + m$ with $0 \le m < q_\nu$ we have also

$$|f(k) - f(k_\nu)| \le \frac{C}{R} m < \frac{C q_\nu}{R} < \frac{CN}{R} \text{ by our bound for } f' \ .$$

Hence

$$|X_\nu - f(k_\nu) \sum_{k_\nu \le k < k_{\nu+1}} \chi(\phi(k))| \le \frac{CN^2}{R} \ , \tag{18}$$

by our definition of X_ν, and since $k_{\nu+1} - k_\nu = q_\nu \le N$. Putting (17) into (18), we see that

$$|X_\nu - f(k_\nu) Y_\nu| \le \frac{CN^2}{R} \ , \qquad \text{with} \tag{19}$$

$$Y_\nu = \sum_{0 \le m < q_\nu} \chi\Big(\xi + \frac{p_\nu}{q_\nu} m + \tau_m\Big) \quad \text{and} \tag{20}$$

$$|\tau_m| \le \frac{C}{N} \ . \tag{21}$$

For each integer n $(0 \le n < q_\nu)$ there is one and only one integer m $(0 \le m < q_\nu)$ for which $\frac{p_\nu}{q_\nu} m \equiv \frac{n}{q_\nu} \mod 1$, since p_ν and q_ν are relatively prime. Let $\tilde{m}(n)$ be that integer m, and define $\tilde{\tau}_n = \tau_{\tilde{m}(n)}$. Since $\chi(\cdot)$ is periodic of period 1, we have

$$\chi\Big(\xi + \frac{p_\nu}{q_\nu} m + \tau_m\Big) = \chi\Big(\xi + \frac{n}{q_\nu} + \tilde{\tau}_n\Big) \text{ for } m = \tilde{m}(n) \ .$$

As n runs from 0 to $q_\nu - 1$, $\tilde{m}(n)$ assumes all the integer values from 0 to $q_\nu - 1$. Hence (20) may be rewritten as

$$(22)\qquad Y_\nu = \sum_{0\le n<q_\nu} \chi\Big(\xi + \frac{n}{q_\nu} + \tilde{\tau}_n\Big)\ , \quad \text{with}$$

$$(23)\qquad |\tilde{\tau}_n| \le \frac{C}{N}\ .$$

Write $\mathrm{Var}_I\,\chi$ for the total variation of χ over an interval I, and write $Av_I\,\chi$ for the mean value of χ on I. Then since $|\tilde{\tau}_n| \le \frac{C}{q_\nu}$ by (23), we have

$$(24)\qquad \Big|\chi\big(\xi + \frac{n}{q_\nu} + \tilde{\tau}_n\big) - Av_{[\xi+\frac{n}{q_\nu},\xi+\frac{(n+1)}{q_\nu}]}\chi\Big| \le \mathrm{Var}_{[\xi+\frac{n-C'}{q_\nu},\xi+\frac{n+C'}{q_\nu}]}\chi$$

for a large C' .

Note that $\sum_{0\le n<q_\nu} \mathrm{Var}_{[\xi+\frac{n-C'}{q_\nu},\xi+\frac{n+C'}{q_\nu}]}\chi \le C''\ \mathrm{Var}_{[0,1]}\chi$ since χ has period 1, and the family of intervals $I_n = \big[\xi + \frac{n-C'}{q_\nu}, \xi + \frac{n+C'}{q_\nu}\big]$ $(0 \le n < q)$ may be divided into C'' families of pairwise disjoint subintervals of the circle $\mathbb{R}/\mathbb{Z}$.

Note also that $\sum_{0\le n<q} Av_{[\xi+\frac{n}{q_\nu},\xi+\frac{(n+1)}{q_\nu}]}\chi = 0$, since χ has period 1 and average zero. Therefore, summing (24) over $n = 0, 1, \dots, q_\nu - 1$ and comparing with (22), we get

$$|Y_\nu| \le C''\ \mathrm{Var}_{[0,1]}\chi \quad \text{for } 0 \le \nu < \nu_{\max}\ .$$

We are assuming $\mathrm{Var}_{[0,1]}\chi \le C$, so

$$|Y_\nu| \le C' \quad \text{for } 0 \le \nu < \nu_{\max}\ .$$

Putting this into (19) and recalling that $N \sim R^{1/3}$, $R \ge 10$, we obtain the estimate

$$(25)\qquad |X_\nu| \le C'' \quad \text{for } 0 \le \nu < \nu_{\max}\ .$$

Estimates (15), (16), (25) show that

$$(26)\qquad \Big|\sum_{0\le k\le S} f(k)\chi(\phi(k))\Big| \le CN + C''\nu_{\max}\ .$$

Let us estimate $\nu_{\max}$. For fixed p, q with $1 \le q \le N$, let $\mathcal{E}(p,q)$ be the set of $\nu < \nu_{\max}$ for which $p_\nu = p$, $q_\nu = q$. Also, let $I_\nu = [k_\nu, k_{\nu+1})$ for $\nu < \nu_{\max}$. The I_ν are pairwise disjoint. For $\nu \in \mathcal{E}(p,q)$ and $t \in I_\nu$ we have

$$\left|\phi'(t) - \frac{p}{q}\right| = \left|\phi'(t) - \frac{p_\nu}{q_\nu}\right| \le \left|\phi'(t) - \phi'(k_\nu)\right| + \left|\phi'(k_\nu) - \frac{p_\nu}{q_\nu}\right|$$
$$\le CR^{-1}|t - k_\nu| + \frac{C}{q_\nu N} \le CR^{-1}q_\nu + \frac{C}{q_\nu N}$$

(since $k_{\nu+1} - k_\nu = q_\nu$) $= CR^{-1}q + \frac{C}{qN}$.

Since $1 \le q \le N \sim R^{1/3}$, we have $R^{-1}q \le \frac{C}{qN}$, and thus $|\phi'(t) - \frac{p}{q}| \le \frac{C'}{qN}$ for $\nu \in \mathcal{E}(p,q)$ and $t \in I_\nu$. Hence the I_ν for $\nu \in \mathcal{E}(p,q)$ are pairwise disjoint subintervals of $F(p,q) = \{t \in [0,S] \mid |\phi'(t) - \frac{p}{q}| \le \frac{C}{qN}\}$. Since $\phi'' > 0$, the set $F(p,q)$ must be a closed interval, say $F(p,q) = [t_{\mathrm{low}}, t_{\mathrm{hi}}]$. Since $\phi'' \ge bR^{-1}$ and $t_{\mathrm{low}}, t_{\mathrm{hi}} \in F(p,q)$, we have $\frac{2C}{qN} \ge \phi'(t_{\mathrm{hi}}) - \phi'(t_{\mathrm{low}}) \ge bR^{-1} \cdot (t_{\mathrm{hi}} - t_{\mathrm{low}})$, i.e. length $(F(p,q)) = t_{\mathrm{hi}} - t_{\mathrm{low}} \le \frac{2CR}{qNb}$.

On the other hand, for $\nu \in \mathcal{E}(p,q)$ the interval I_ν has length $k_{\nu+1} - k_\nu = q_\nu = q$. So the I_ν for $\nu \in \mathcal{E}(p,q)$ are pairwise disjoint intervals of length q, all contained in an interval $F(p,q)$ of length at most $\frac{2CR}{qNb}$. Consequently, there can be at most $\frac{2CR}{q^2Nb}$ distinct ν in $\mathcal{E}(p,q)$.

For a given q, $(1 \le q \le N)$, how many p can have $\mathcal{E}(p,q)$ non-empty? Since $0 < \phi'' \le CR^{-1}$ and $[0,S]$ has length $S \le R$, it follows that $\phi'(t)$ varies by at most C, as t varies over $[0,S]$. If $\nu \in \mathcal{E}(p,q)$ and $\tilde{\nu} \in \mathcal{E}(\tilde{p},q)$, then $|\phi'(k_\nu) - \frac{p}{q}| = |\phi'(k_\nu) - \frac{p_\nu}{q_\nu}| \le \frac{C}{q_\nu N} = \frac{C}{qN}$, and similarly $|\phi'(k_{\tilde{\nu}}) - \frac{\tilde{p}}{q}| \le \frac{C}{qN}$. We know that $|\phi'(k_\nu) - \phi'(k_{\tilde{\nu}})| \le C$, so we must have $|p - \tilde{p}| \le Cq$. So for a given q we find that $\mathcal{E}(p,q)$ can be non-empty for at most Cq distinct p. Combining this with our bound for the number of ν in a given $\mathcal{E}(p,q)$, we see that $\bigcup\limits_p \mathcal{E}(p,q)$ contains at most $\frac{C'R}{qNb}$ distinct ν. Since $\{0, q, \ldots, \nu_{\max} - 1\} = \bigcup\limits_{1 \le q \le N} \left(\bigcup\limits_p \mathcal{E}(p,q)\right)$, it follows that

$\nu_{\max} \le \sum_{1\le q\le N} \frac{C'R}{qNb} \le \frac{C''R\ell nN}{Nb}$. Hence, (26) implies the estimate

$$\Big|\sum_{0\le k\le S} f(k)\chi(\phi(k))\Big| \le CN + \frac{CR\ell nN}{Nb} .$$

Since $N \sim R^{1/3}$ and $b \le C$, the right-hand side is comparable to $\frac{CR^{2/3}\ell nR}{b}$, which proves the conclusion of the Lemma. ■

Trivial Remarks. In place of $bR^{-1} \le \phi''(t) \le CR^{-1}$ in the above Lemma, we could just as easily assume $bR^{-1} \le -\phi''(t) \le CR^{-1}$ for $t \in [0,S]$. Also, we can replace $[0,S]$ by any other interval of length $\le R$.

To prove (7), (8), (9) we will use Lemma 1 with

(26bis) $$\phi(t) = \frac{1}{\pi}\int_0^\infty \Big(-V(r) - \frac{t(t+1)}{r^2}\Big)_+^{1/2} dr - \frac{1}{2}\ ,\ 0 < t < \Omega\ .$$

Thus, $\phi_\ell = \phi(\ell)$. To apply lemma 1, we need upper and lower bounds for $\phi''(t)$, which we now establish. We set

$$\Phi(\xi) = \frac{1}{\pi}\int_0^\infty \big(-V(r) - \frac{\xi}{r^2}\big)_+^{1/2} dr - \frac{1}{2}\ ,$$

so that

(27) $$\Phi'(\xi) = -\frac{1}{2\pi}\int_0^\infty \big(-r^2V(r) - \xi\big)_+^{-1/2}\frac{dr}{r}\ .$$

We recall the following properties of $r^2V(r)$.

(28) $$\Big|\big(\frac{d}{dr}\big)^\alpha\big(-r^2V(r)\big)\Big| \le C_\alpha \mathcal{S}(r) r^{-\alpha} \quad \text{with } \mathcal{S}(r) = \min\{Zr, r^{-2}\}\ ,$$

(29) $-r^2V(r)$ has a maximum at $r = \check{r} \sim Z^{-1/3}$, and

(30) $$-\frac{d^2}{dr^2}\big(-r^2V(r)\big) \ge c\mathcal{S}(r)r^{-2} \text{ at } r = \check{r}\ .$$

Moreover, given $c_1 > 0$, we have

$$(31) \qquad \Big|\Big(\frac{d}{dr}\Big)\big(-r^2V(r)\big)\Big| > c_2\mathcal{S}(r)r^{-1}\text{for } |r-\check{r}| > c_1\check{r}\ ,$$

with $c_2 > 0$ depending on c_1. We introduce a partition of unity $\sum_\nu \theta_\nu(r) = 1$ on $(0,\infty)$, with θ_ν supported in $\{|r-r_\nu| < cr_\nu\}$, $r_{\nu+1}/r_\nu > 1+c'$, $\big|\big(\frac{d}{dr}\big)^\alpha\theta_\nu\big| \le C_\alpha r_\nu^{-\alpha}$; and then write

$$(32) \qquad \Phi'(\xi) = -\sum_\nu \int_0^\infty \big(-r^2V(r)-\xi\big)_+^{-1/2}\theta_\nu(r)\frac{dr}{2\pi r} \equiv -\sum_\nu Q_\nu(\xi)\ .$$

Lemma 9 from the section on the Eigenvalue Sum in an Approximate TF Potential with an Exact Coulomb singularity applies here, so that we get the following estimates for $Q_\nu(\xi)$.

$$(33) \quad \Big|\Big(\frac{d}{d\xi}\Big)^m Q_\nu(\xi)\Big| \le C_m\mathcal{S}^{-\frac{1}{2}-m}(r_\nu) \text{ for } 0<\xi<C\mathcal{S}(r_\nu)\ ,$$
$$\text{provided } \operatorname{dist}(\check{r},\ \operatorname{supp}\theta_\nu) > c\check{r}\ .$$

$$(34) \quad \Big|\Big(\frac{d}{d\xi}\Big)^m Q_\nu(\xi)\Big| \le C_m\mathcal{S}^{-\frac{1}{2}-m}(r_\nu) \text{ for } 0<\xi<\max_{r>0}[-r^2V(r)]\ ,$$
$$\text{provided } \operatorname{dist}(\check{r},\ \operatorname{supp}\theta_\nu) \le c\check{r}\ .$$

Immediately from the definition of Q_ν we have

$$(35) \qquad Q_\nu(\xi) = 0 \text{ for } \xi > C\mathcal{S}(r_\nu)\ .$$

Combining (33), (34), (35), we find that

$$(36) \qquad \Big|\Big(\frac{d}{d\xi}\Big)^m Q_\nu(\xi)\Big| \le C_m\mathcal{S}^{-\frac{1}{2}-m}(r_\nu) \quad \text{for } 0<\xi<\max_{r>0}[-r^2V(r)]\ .$$

Putting (35) and (36) into (32), we obtain for $0<\xi<\max_{r>0}[-r^2V(r)]$ that

$$\Big|\Big(\frac{d}{d\xi}\Big)^m\Phi'(\xi)\Big| \le C_m \sum_{C\mathcal{S}(r_\nu)>\xi} \mathcal{S}^{-\frac{1}{2}-m}(r_\nu)$$
$$\sim \sum_{\substack{CZr_\nu>\xi\\ r_\nu\le Z^{-1/3}}} (Zr_\nu)^{-\frac{1}{2}-m} + \sum_{\substack{Cr_\nu^{-2}>\xi\\ r_\nu>Z^{-1/3}}} (r_\nu^{-2})^{-\frac{1}{2}-m}\ ,$$

i.e.

$$(37)\qquad \Big|\Big(\frac{d}{d\xi}\Big)^m \Phi'(\xi)\Big| \le C_m \xi^{-\frac{1}{2}-m} \text{ for } 0<\xi<\max_{r>0}[-r^2V(r)]\ ,\ m\ge 0\ .$$

Upper and lower bounds for $\phi''(t)$ come from (37), (11) and the close relation among $\phi(t)$, $\Phi(\xi)$, $\Theta(t)$. In fact, $\phi(t)=\Phi(t(t+1))$, so

$$\phi''(t)=(2t+1)^2\Phi''(t(t+1))+2\Phi'(t(t+1))\ .$$

Hence, (37) yields

$$|\phi''(t)|\le C(2t+1)^2[t(t+1)]^{-3/2}+C[t(t+1)]^{-1/2} \text{ for } 0<t<\Omega\ .$$

In particular,

$$(38)\qquad |\phi''(t)|\le \frac{C}{t} \quad \text{for } 1<t<\Omega\ .$$

Similarly, $\Theta(t)=\pi\Phi(t^2)+\frac{\pi}{2}$, so for $0<t<[\max_{r>0}\big(-r^2V(r)\big)]^{1/2}$ we get from (37) that

$$(39)\qquad |\Theta'(t)|=|2\pi t\Phi'(t^2)|\le(2\pi t)\cdot C[t^2]^{-1/2}\le C'\ .$$

Also, $\phi(t)=\frac{1}{\pi}\Theta(\sqrt{t(t+1)})-\frac{1}{2}=\frac{1}{\pi}\Theta(H(t))-\frac{1}{2}$ with $H(t)=\sqrt{t(t+1)}$, so

$$(40)\qquad \phi''(t)=\frac{1}{\pi}(H'(t))^2\Theta''(H(t))+\frac{1}{\pi}H''\Theta'(H(t)) \text{ for } 0<t<\Omega\ .$$

For $t>100$ we have $H(t)=\sqrt{t(t+1)}=t+\frac{1}{2}+\sum_{k\ge1}c_kt^{-k}$ (convergent power series), so $H'(t)\sim 1$ and $|H''(t)|\le Ct^{-3}$. Hence (40) implies

$$(41)\qquad |\phi''(t)|\ge c|\Theta''(H(t))|-Ct^{-3}|\Theta'(H(t))| \quad \text{for } 100<t<\Omega\ .$$

Putting (11) and (39) into (41), we see that

$$|\phi''(t)|\ge cZ^{-\frac{1}{3}}-Ct^{-3} \text{ for } Z^{10^{-9}}<t<\Omega\ .$$

In particular,

$$|\phi''(t)| \geq c' Z^{-\frac{1}{3}} \quad \text{for } C' Z^{\frac{1}{9}} < t < \Omega \ . \tag{42}$$

Thus we have derived both upper and lower bounds for $|\phi''|$, namely (38) and (42).

To prove (8) we can take $f(t) \equiv 1$ in Lemma 1. To prove (7), (9) we need instead

$$f(t) = (2t+1)\Big[\int_0^\infty \big(-V(r) - \frac{t(t+1)}{r^2}\big)_+^{-1/2} dr\Big]^{-1} \ . \tag{43}$$

Hence we must estimate $f(t)$ and $f'(t)$ for $0 < t < \Omega$. Define

$$n_1(\xi) = \int_0^\infty \Big(-V(r) - \frac{\xi}{r^2}\Big)_+^{-1/2} dr \ . \tag{44}$$

Using the partition of unity θ_ν appearing in (32), we write

$$n_1(\xi) = \sum_\nu \int_0^\infty \big(-r^2 V(r) - \xi\big)_+^{-1/2} r\theta_\nu(r) dr \equiv \sum_\nu P_\nu(\xi) \ . \tag{45}$$

Again using Lemma 9 from the section on the Eigenvalue Sum in an Approximate TF Potential with an Exact Coulomb Singularity, we learn that

$$\big|\big(\frac{d}{d\xi}\big)^m P_\nu(\xi)\big| \leq C_m \mathcal{S}^{-\frac{1}{2}-m}(r_\nu)\cdot r_\nu^2 \quad \text{for } 0 < \xi < C\mathcal{S}(r_\nu) \ , \tag{46}$$

$$\text{provided } \ \operatorname{dist}(\check{r}, \ \operatorname{supp} \theta_\nu) > c\check{r}$$

$$\big|\big(\frac{d}{d\xi}\big)^m P_\nu(\xi)\big| \leq C_m \mathcal{S}^{-\frac{1}{2}-m}(r_\nu)\cdot r_\nu^2 \text{ for } 0 < \xi < \max_{r>0}[-r^2 V(r)] \tag{47}$$

$$\text{provided } \operatorname{dist}(\check{r}, \ \operatorname{supp} \theta_\nu) \leq c\check{r} \ .$$

Immediately from the definition we get

$$P_\nu(\xi) = 0 \quad \text{for} \quad \xi > C\mathcal{S}(r_\nu) \ . \tag{48}$$

Combining (46)...(48), we get

$$\big|\big(\frac{d}{d\xi}\big)^m P_\nu(\xi)\big| \leq C_m \mathcal{S}^{-\frac{1}{2}-m}(r_\nu)\cdot r_\nu^2 \chi_{CS(r_\nu)>\xi} \text{ for } 0 < \xi < \max_{r>0}[-r^2 V(r)] \ . \tag{49}$$

Putting (49) into (45) yields

$$(50)\quad \big|\big(\frac{d}{d\xi}\big)^m n_1(\xi)\big| \le C_m \sum_{C\mathcal{S}(r_\nu)>\xi} r_\nu^2 \mathcal{S}^{-\frac{1}{2}-m}(r_\nu)$$

$$\sim \sum_{\substack{CZr_\nu>\xi \\ r_\nu<Z^{-1/3}}} r_\nu^2 (Zr_\nu)^{-\frac{1}{2}-m} + \sum_{\substack{Cr_\nu^{-2}>\xi \\ r_\nu\ge Z^{-1/3}}} r_\nu^2 (r_\nu^{-2})^{-\frac{1}{2}-m} .$$

The first sum on the right has the order of magnitude

$$(Z^{-\frac{1}{3}})^2 \cdot (Z \cdot Z^{-\frac{1}{3}})^{-\frac{1}{2}-m} = Z^{-\frac{2}{3}} \cdot Z^{-\frac{1}{3}-\frac{2}{3}m} = Z^{-1-\frac{2}{3}m}$$

for $m = 0, 1$.

The second sum on the right has the order of magnitude $(\xi^{-1/2})^2 \cdot (\xi)^{-\frac{1}{2}-m} = \xi^{-\frac{3}{2}-m}$. The second term $\xi^{-\frac{3}{2}-m}$ dominates the first term $Z^{-1-\frac{2}{3}m}$ since $0 < \xi < \max_{r>0}[-r^2 V(r)] \sim Z^{2/3}$. Therefore (50) implies

$$(51)\quad n_1(\xi) \le C\xi^{-3/2} \text{ for } 0 < \xi < \max_{r>0}[-r^2 V(r)] ,$$

and

$$(52)\quad \big|\big(\frac{d}{d\xi}\big) n_1(\xi)\big| \le C\xi^{-5/2} \text{ for } 0 < \xi < \max_{r>0}[-r^2 V(r)] .$$

Next, set $n_2(t) = \int_0^\infty \big(-V(r) - \frac{t(t+1)}{r^2}\big)_+^{-1/2} dr = n_1(t(t+1))$ for $0 < t < \Omega$. Estimates (51), (52) for n_1 show that

$$(53)\quad n_2(t) \le C(t(t+1))^{-3/2} \le C' t^{-3} \quad \text{for } 1 \le t < \Omega \text{ , and}$$

$$(54)\quad \big|\big(\frac{d}{dt}\big) n_2(t)\big| \le (2t+1) \cdot C(t(t+1))^{-5/2} \le C' t^{-4} \text{ for } 1 \le t < \Omega .$$

We derive a lower bound for $n_2(t)$ by using equations (3)...(15) in the section on Approximate TF Potentials. These estimates hold for integers ℓ, $1 \le \ell < \Omega$.

If $1 \le \ell < (1 - \overline{c})\Omega$, then we know that from (3)...(15) that

$$0 < -V(r) - \frac{\ell(\ell+1)}{r^2} < -V(r) \le C \min\{\frac{Z}{r}, r^{-4}\}$$

for $r \in (x_{\text{left}}(\ell), x_{\text{rt}}(\ell))$, and that $\ell^{-1} \sim x_{\text{rt}}(\ell) > (1+c')x_{\text{left}}(\ell)$. Therefore,

$$(55) \quad n_2(\ell) \geq \int_{x_{\text{left}}(\ell)}^{x_{\text{rt}}(\ell)} c \cdot \Big[\min\{\frac{Z}{r}, r^{-4}\}\Big]^{-1/2} dr \geq c \int_{(1+c')^{-1}x_{\text{rt}}(\ell)}^{x_{\text{rt}}(\ell)} r^2 dr$$
$$\geq c''(x_{\text{rt}}(\ell))^3 \geq c'''\ell^{-3} \ .$$

On the other hand, if $(1-\overline{c})\Omega \leq \ell < \Omega$, then we know from (3)...(15) that $V_\ell(r) = \frac{\ell(\ell+1)}{r^2} + V(r)$ has a minimum at $r = x_0(\ell) \sim Z^{-1/3}$, and that

$$-V_\ell(x_0(\ell)) \sim \frac{\Omega(\Omega-\ell)}{[x_0(\ell)]^2} \sim Z(\Omega-\ell)$$
$$V_\ell'(x_0(\ell)) = 0$$
$$V_\ell'' \sim \frac{Z}{x_0(\ell)} \cdot [x_0(\ell)]^{-2} \sim Z^2 \quad \text{for } |x - x_0(\ell)| < c_2 x_0(\ell) \sim Z^{-1/3} \ .$$

It follows that $-V_\ell(x) \sim Z \cdot (\Omega - \ell)$ for $|x - x_0(\ell)| < c_3\big(\frac{\Omega-\ell}{Z}\big)^{1/2}$, provided c_3 is taken small enough. Consequently

$$n_2(\ell) = \int_0^\infty \big(-V_\ell(r)\big)_+^{-1/2} dr \geq c \int_{|x-x_0(\ell)|<c_3(\frac{\Omega-\ell}{Z})^{1/2}} [Z\cdot(\Omega-\ell)]^{-1/2} dx$$
$$\sim \big(\frac{\Omega-\ell}{Z}\big)^{1/2} \cdot \frac{1}{[Z(\Omega-\ell)]^{1/2}} \sim \frac{1}{Z} \sim \ell^{-3}$$
$$(\text{since } (1-\overline{c})\Omega \leq \ell < \Omega) \ .$$

Combining this with (55), we obtain $n_2(\ell) \geq c\ell^{-3}$ for integers ℓ with $1 \leq \ell < \Omega$. Estimate (54) then implies

$$(56) \qquad n_2(t) \geq ct^{-3} \quad \text{for } C \leq t < \Omega \ .$$

Now we can estimate $f(t)$ as in (43). By definition of f, $n_2(\cdot)$ we have

$$f(t) = \frac{(2t+1)}{n_2(t)} \ .$$

Therefore (53), (54), (56) imply

$$(57) \quad f(t) \sim t^4 \quad \text{for } C \leq t < \Omega \ , \quad \text{and}$$
$$|f'(t)| = \Big|\frac{2}{n_2(t)} - \frac{(2t+1)n_2'(t)}{(n_2(t))^2}\Big| \leq \frac{C}{t^{-3}} + \frac{C(2t+1)t^{-4}}{(t^{-3})^2} \ ,$$

i.e.

$$|f'(t)| \le C' t^3 \quad \text{for } C \le t < \Omega\ . \tag{58}$$

Note that $n_2(\ell) = n_\ell$ for integers ℓ, so (53) and (56) imply

$$n_\ell \sim \ell^{-3} \quad \text{for } C \le \ell < \Omega\ . \tag{59}$$

We are ready to prove (7), (8), (9) with $a = \frac{1}{50}$. Suppose we are given $L_1 < L_2 < \Omega$, with $L_1 > CZ^{1/9}$ and $L_1 > cL_2$. Then the phase function $\phi(t)$ in (26 bis) satisfies

$$cZ^{-1/3} \le |\phi''(t)| \le C(L_2)^{-1} \quad \text{in } [L_1, L_2]\ ,$$

by virtue of (38) and (42).

Thus, $\phi(t)$ on $[L_1, L_2]$ satisfies the hypotheses of Lemma 1, with $R = L_2$, $b = L_2 Z^{-1/3}$, $S = L_2 - L_1 \le R$. We take $\chi(t)$ in Lemma 1 to be $\chi_-(t)$, and note that it has period 1, average zero, and bounded variation on $[0,1]$. Thus, χ satisfies the hypotheses of Lemma 1. For $f(t)$ we take the function (43). Estimates (57), (58) show that $(L_2)^{-4} f(t)$ satisfies the hypotheses of Lemma 1 on $[L_1, L_2]$.

Therefore, Lemma 1 applies, and it tells us that

$$\Big| \sum_{L_1 \le \ell \le L_2} \frac{f(\ell)}{(L_2)^4} \chi_-(\phi(\ell)) \Big| \le \frac{C}{b} R^{2/3} \ell n R\ , \quad \text{i.e.}$$

$$\Big| \sum_{L_1 \le \ell \le L_2} \frac{(2\ell+1)}{n_\ell} \chi_-(\phi_\ell) \Big| \le \frac{C}{L_2 Z^{-1/3}} (L_2^{2/3} \ell n L_2) \cdot L_2^4\ , \quad \text{i.e.}$$

$$\Big| \sum_{L_1 \le \ell \le L_2} \frac{(2\ell+1)}{n_\ell} \chi_-(\phi_\ell) \Big| \le C Z^{1/3} L_2^{\frac{11}{3}} \ell n Z$$

$$\text{for} \quad CZ^{1/9} \le L_1 < L_2 < \Omega \text{ with } L_1 > cL_2\ . \tag{60}$$

Similarly, taking $\tilde\chi$ in place of χ_- above, we get

$$\Big| \sum_{L_1 \le \ell \le L_2} \frac{(2\ell+1)}{n_\ell} \tilde\chi(\phi_\ell) \Big| \le C Z^{1/3} L_2^{11/3} \ell n Z \tag{61}$$

$$\text{for} \quad CZ^{1/9} \le L_1 < L_2 < \Omega \text{ with } L_1 > cL_2\ .$$

Estimate (61) easily implies (9). In fact, we divide the integers ℓ between $Z^{\frac{8}{25}+10\varepsilon}$ and Ω into disjoint intervals $\{L_1^\nu \leq \ell \leq L_2^\nu\}$ with L_2^ν/L_1^ν between 2 and 3.

Applying (61) to each of these intervals and summing on ν, we obtain

$$\Big| \sum_{Z^{\frac{8}{25}+10\varepsilon} < \ell < \Omega} \frac{(2\ell+1)}{n_\ell} \tilde{\chi}(\phi_\ell) \Big| \leq C Z^{1/3} \Omega^{\frac{11}{3}} \ell n Z \leq C' Z^{\frac{14}{9}} \ell n Z \ . \tag{62}$$

Thus, (9) holds provided $Z^{\frac{14}{9}} \ell n Z < C\Omega^{-2a} Z^{\frac{5}{3}}$, i.e. provided $a < \frac{1}{6}$.

Similarly, (60) implies (7) with $a = \frac{1}{50}$. In fact, suppose we are given integers ℓ_1, ℓ_2 satisfying

$$Z^{10^{-9}} \leq \ell_1 < \ell_2 < \Omega \ , \quad \text{and} \quad \ell_2 - \ell_1 > \Omega^{1-10a} \ . \tag{63}$$

Then $\ell_2 > \Omega^{1-10a} \sim (Z^{1/3})^{4/5} >> Z^{1/9}$. Assume for a moment that $\ell_1 \geq c\ell_2$. Then (60) applies, with ℓ_1, ℓ_2 in place of L_1, L_2. Hence,

$$\Big| \sum_{\ell_1 \leq \ell \leq \ell_2} \frac{(2\ell+1)}{n_\ell} \chi_-(\phi_\ell) \Big| \leq C Z^{1/3} \ell_2^{\frac{11}{3}} \ell n Z \ .$$

On the other hand, (59) and $\ell_1 \geq c\ell_2$ show that

$$\Omega^{-2a} \sum_{\ell_1 \leq \ell \leq \ell_2} \frac{(2\ell+1)}{n_\ell} \sim \Omega^{-2a} \cdot \ell_2^4 \cdot (\ell_2 - \ell_1) \ .$$

Consequently, (7) holds, provided $Z^{\frac{1}{3}} \ell_2^{\frac{11}{3}} \ell n Z \leq C\Omega^{-2a} \ell_2^4 (\ell_2 - \ell_1)$, i.e. $Z^{1/3} \ell n Z \leq C\Omega^{-2a} \ell_2^{1/3} (\ell_2 - \ell_1)$. This in turn follows from $Z^{1/3} \ell n Z \leq C\Omega^{-2a} (\ell_2 - \ell_1)^{4/3}$, which is a consequence of $Z^{\frac{1}{3}} \ell n Z \leq C\Omega^{-2a} (\Omega^{1-10a})^{\frac{4}{3}}$, i.e. $Z^{\frac{1}{3}} \ell n Z \leq C\Omega^{\frac{4}{3} - \frac{46}{3} a}$, which is true for $a = \frac{1}{50}$. Therefore, (7) holds with $a = \frac{1}{50}$, provided $\ell_1 \geq c\ell_2$. On the other hand, assume (63) with $\ell_1 < c\ell_2$. Subdivide the integers between ℓ_1 and ℓ_2 into pairwise disjoint intervals $\{\ell_1^\nu \leq \ell \leq \ell_2^\nu\}$ with ℓ_2^ν/ℓ_2^ν between 2 and 3.

If $\ell_1^\nu > CZ^{1/9}$, then (60) yields

$$\Big| \sum_{\ell_1^\nu \leq \ell \leq \ell_2^\nu} \frac{(2\ell+1)}{n_\ell} \chi_-(\phi_\ell) \Big| \leq C Z^{\frac{1}{3}} (\ell_2^\nu)^{\frac{11}{3}} \ell n Z \ . \tag{64}$$

If instead $\ell_1^\nu \le CZ^{1/9}$, then we use (59) to make the trivial estimate

$$\Big| \sum_{\ell_1^\nu \le \ell \le \ell_2^\nu} \frac{(2\ell+1)}{n_\ell} \chi_-(\phi_\ell) \Big| \le C \sum_{\ell_1^\nu \le \ell \le \ell_2^\nu} \frac{(2\ell+1)}{n_\ell} \le C'(\ell_2^\nu)^5 \ . \tag{65}$$

Summing (64), (65) over ν, we get

$$\Big| \sum_{\ell_1 \le \ell \le \ell_2} \frac{(2\ell+1)}{n_\ell} \chi_-(\phi_\ell) \Big| \le CZ^{\frac{1}{3}} (\ell_2)^{\frac{11}{3}} \ell n Z + CZ^{5/9} \ . \tag{66}$$

On the other hand, (59) and $\ell_1 \le c\ell_2$ imply

$$\sum_{\ell_1 \le \ell \le \ell_2} \frac{(2\ell+1)}{n_\ell} \sim \sum_{\ell_1 \le \ell \le \ell_2} \ell^4 \sim \ell_2^5 \ .$$

Hence, (7) holds, provided

$$Z^{\frac{1}{3}} \ell_2^{\frac{11}{3}} \ell n Z + Z^{\frac{5}{9}} \le C\Omega^{-2a} \ell_2^5 \ , \quad \text{i.e.} \tag{67}$$

$$Z^{\frac{1}{3}} \ell n Z \le C\Omega^{-2a} \ell_2^{\frac{4}{3}} \quad \text{and} \quad Z^{\frac{5}{9}} \le C\Omega^{-2a} \ell_2^5 \ . \tag{68}$$

Since $\ell_2 > \ell_2 - \ell_1 > \Omega^{1-10a}$ and $a = \frac{1}{50}$, we have

$$\Omega^{-2a} \ell_2^{4/3} > \Omega^{-2a} \Omega^{\frac{4}{3} - \frac{40a}{3}} = \Omega^{\frac{4}{3} - \frac{46}{3}a} > \Omega \, \ell n \, \Omega > cZ^{1/3} \ell n Z$$

and

$$\Omega^{-2a} \ell_2^5 > \Omega^{-2a} \Omega^{5-50a} = \Omega^{4-2a} > Z^{\frac{5}{9}} \ .$$

Thus, (68) holds, and therefore (7) is valid also for $\ell_1 \le c\ell_2$. Hence, (7) holds with $a = \frac{1}{50}$ in all cases.

Next we prove (8). For $\Omega \ge 2L > CZ^{1/9}$, and $\phi(t)$ given by (26 bis) we know that

$$cZ^{-1/3} \le |\phi''(t)| \le \frac{C}{L} \quad \text{for } t \in [L, 2L], \quad \text{by virtue of (38), (42)} \ .$$

Thus, $\phi(t)$ satisfies the hypotheses of Lemma 1 with $R = S = L$, $b = Z^{-1/3}L$. For $\chi(t)$ we take the function

$$\chi(t) = \begin{cases} 1 - \tilde{c}L^{-6/43} & \text{if } |t - \text{ nearest integer}| \le 10L^{-6/43} \\ -\tilde{c}L^{-6/43} & \text{otherwise} \ . \end{cases}$$

This function has period 1 and bounded variation on $[0,1]$; and for a suitable $\tilde{c} \sim 1$, $\chi(t)$ has average zero. Therefore, $\chi(t)$ satisfies the hypotheses of Lemma 1.

For $f(t)$ in Lemma 1, we just take $f(t) \equiv 1$. Thus, all the hypotheses of Lemma 1 are satisfied. Applying the Lemma, we learn that

$$\Big|\big[\text{Number of } \ell \in [L,2L] \text{ with } |\phi_\ell - \text{ nearest integer}| \le 10L^{-6/43}\big] - \tilde{c}L^{-6/43}\cdot L\Big| \le \frac{CL^{2/3}\ell n L}{Z^{-\frac{1}{3}}L} \le \frac{C'Z^{1/3}\ell n Z}{L^{1/3}} .$$

Therefore, the number of $\ell \in [L,2L]$ with $|\phi_\ell - \text{nearest integer}| \le \ell^{-6/43}$ is at most $\tilde{c}L^{\frac{37}{43}} + \frac{C'Z^{1/3}\ell n Z}{L^{1/3}}$. We know this for $CZ^{1/9} \le 2L < \Omega$.

Let us apply the above estimate for $L = L_m \equiv 2^{-m}\cdot(\Omega/2)$ and $m = 0,1,\dots,m_{\max}$ with $m_{\max}$ taken so that $L_{m_{\max}} \sim Z^{\frac{1}{4}}$. Summing on m, we see that

$$\begin{aligned}&(\text{Number of } \ell \in [Z^{\frac{1}{4}},\Omega) \text{ with } |\phi_\ell - \text{ nearest integer}| \le \ell^{-6/43})\\ &\qquad \le \sum_{m=0}^{m_{\max}} \big(\tilde{c}L_m^{\frac{37}{43}} + C'Z^{1/3}\frac{\ell n Z}{L_m^{1/3}}\big) + C \sim \Omega^{\frac{37}{43}} + \frac{Z^{1/3}\ell n Z}{Z^{1/12}} \sim \Omega^{\frac{37}{43}} .\end{aligned}$$

Combining this with the trivial estimate

$$(\text{Number of } \ell \le Z^{1/4} \text{ with } |\phi_\ell - \text{nearest integer}| \le \ell^{-6/43}) \le Z^{1/4} << \Omega^{\frac{37}{43}} ,$$

we obtain

$$\begin{aligned}&(\text{Number of } \ell < \Omega \text{ with } |\phi_\ell - \text{ nearest integer}| \le \ell^{-6/43}) < C\Omega^{\frac{37}{43}}\\ &\qquad \le C\Omega^{1-6a} \quad \text{for } a \le \frac{1}{43} .\end{aligned}$$

Thus, (8) holds, provided $a \le \frac{1}{43}$. The following result summarizes our knowledge of (7), (8), (9).

Lemma 2. *Assume $V(r)$ satisfies (1), (2), (3), (11). Set $a = 1/50$.*

(A) *Given ℓ_1, ℓ_2 integers, with $Z^{10^{-9}} \le \ell_1 < \ell_2 < \Omega$ and $\ell_2 - \ell_1 > \Omega^{1-10a}$, we have*

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

(B) *There are at most* $C\Omega^{1-6a}$ *integers* $\ell < \Omega$ *for which* $|\phi_\ell -$ *nearest integer*$| \leq \ell^{-6/43}$.

(C)

$$\Big| \sum_{Z^{\frac{8}{25}+10\varepsilon}<\ell<\Omega} \frac{(2\ell+1)}{n_\ell} \tilde{\chi}(\phi_\ell) \Big| \leq C\Omega^{-2a} Z^{5/3} \ .$$

This lets us make use of our previous results on the density and eigenvalue sum for $-\Delta + V$. We spell out the conclusions in the next section.

The Main Theorems for Approximate TF Potentials

Recall that $V_Z^{TF}(x)$ denotes the screened Thomas-Fermi potential on $\mathbb{R}^3$. Thus, $-\Delta V_Z^{TF} = (\text{const})(-V_Z^{TF})^{3/2}$ on $\mathbb{R}^3 \backslash \{0\}$, and $V_Z^{TF}(x) = -\frac{Z}{|x|} + O(Z^{4/3})$ as $x \to 0$. Write $V_Z^{TF}(r)$ for the corresponding function on $(0,\infty)$.

Suppose $V(r)$ is a real-valued function on $(0,\infty)$. Assume the following estimates.

(1) $$\left|\left(\frac{d}{dr}\right)^{\alpha} V(r)\right| \le C_\alpha \min\left\{\frac{Z}{r}, r^{-4}\right\} \cdot r^{-\alpha} \quad \text{for } r>0\ , \alpha \ge 0\ .$$

(2) $$\left|\left(\frac{d}{dr}\right)^{\alpha} \left\{V(r) - V_Z^{TF}(r)\right\}\right| \le c_0 \min\left\{\frac{Z}{r}, r^{-4}\right\} \cdot r^{-\alpha} \quad \text{for } r>0\ ,\ 0 \le \alpha \le 2$$

with $c_0 > 0$ determined by the C_α in (1) .

(3) $$\left|\left(\frac{d}{dr}\right)^{\alpha} \left\{E_0 - \frac{Z}{r} - V(r)\right\}\right| \le C_\alpha Z^{3/2} r^{\frac{1}{2}-\alpha} \quad \text{for } \alpha \ge 0\ ,\ 0 < r < Z^{-\frac{3}{5}+2\cdot 10^{-12}}\ .$$

Define $\Theta(t) = \int_0^\infty \left(-V(r) - \frac{t^2}{r^2}\right)_+^{1/2} dr$, and assume

(4) $$\left|\frac{d^2\Theta(t)}{dt^2}\right| \ge cZ^{-1/3} \quad \text{for } Z^{10^{-9}} < t < \left[\max_{r>0}\left(-r^2 V(r)\right)\right]^{1/2}\ .$$

Let $H = -\Delta + V(|x|)$ on $\mathbb{R}^3$, and let $E_1 \dots E_N$, $\varphi_1(x) \dots \varphi_N(x)$ be the non-positive eigenvalues of H and their corresponding normalized eigenfunctions. Define $\text{sneg}(H) = E_1 + \ldots + E_N$,

$$\rho(x) = \sum_{k=1}^{N} |\varphi_k(x)|^2 \quad \text{for } x \in \mathbb{R}^3\ ,$$
$$\rho_{sc}(x) = \frac{1}{6\pi^2}\left(-V(x)\right)^{3/2} \quad \text{for } x \in \mathbb{R}^3\ .$$

Then we have the following result.

Main Theorem. *If (1)... (4) hold, then*

$$\int_{\mathbb{R}^3 \times \mathbb{R}^3} [\rho(x) - \rho_{sc}(x)] \cdot [\rho(y) - \rho_{sc}(y)] \frac{dxdy}{|x-y|} \le C' Z^{\frac{5}{3}-\frac{1}{75}}$$

and

$$\operatorname{sneg}(H) = -\frac{1}{15\pi^2}\int_{\mathbb{R}^3}\big(-V(x)\big)^{5/2}dx+\frac{Z^2}{8}+\frac{1}{48\pi^2}\int_{\mathbb{R}^3}(\Delta V(x))\cdot\big(-V(x)\big)^{1/2}dx+\text{ Error },$$

with $|\text{Error}| \leq C' Z^{\frac{5}{3}-\frac{1}{75}}$.

Proof. The first conclusion follows from Lemma 2 in the previous section, and from Theorem 2 in the section on the Density for an Approximate TF Potential.

The second conclusion follows from Lemma 2 in the previous section, and from the WKB Eigenvalue Sum Theorem for Approximate TF Potentials. ■

Remark. By using [CFS] in place of Lemma 2, one obtains a sharper bound for the error in the formula for $\operatorname{sneg}(-\Delta + V_{TF}^{Z})$.

References

[B] V. Bach, *Error Bound for the Hartree-Fock Energy of Atoms and Molecules,*, Comm. Math. Phys..

[CFS] A. Cordoba, C. Fefferman, and L. Seco, (to appear).

[FS1] C. Fefferman and L. Seco, *The Ground-State Energy of a Large Atom*, Bull. A.M.S. **23**; no 2 (1990), 525–530.

[FS2] ———, *Eigenvalues and Eigenfunctions of Ordinary Differential Operators*, Advances in Math **95** (1992), 145–305.

[FS3] ———, *On the Dirac and Schwinger Corrections to the Ground-State Energy of an Atom*, Advances in Math (to appear).

[FS4] ———, *The Density in a One-Dimensional Potential*, Advances in Math (to appear).

[FS5] ———, *The Eigenvalue Sum for a One-Dimensional Potential*, Advances in Math (to appear).

[FS6] ———, *Aperiodicity of the Hamiltonian Flow in the Thomas-Fermi Potential*, Rev. Math. Iberoam. (to appear).

[GS] G.-M. Graf and J. Solovej (to appear).

[FS7] ———, *The Density in a Three-Dimensional Radial Potential*, Advances in Math (to appear).

[Hi] E. Hille, *On the Thomas-Fermi Equation*, Proc. Nat. Acad. Sci. USA **62**, 7–10.

[Hu] W. Hughes, *An Atomic Energy Lower Bound that Agrees with Scott's Corrections*, Advances in Math **79** (1990), 213–270.

[L] E. Lieb, *Thomas-Fermi and Related Theories of Atoms and Molecules*, Rev. Mod. Phys. **53**; no. 4; part I (1981), 603–641.