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RAFAEL BENGURIA
STEFAN HOOPS
HEINZ SIEDENTOP

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Bounds on the excess charge and the ionization energy for the Hellmann-Weizsäcker model

by

Rafael BENGURIA
Facultad de Física, P. Universidad Católica de Chile,
Avda. Vicuña Mackenna 4860,
Casilla 306, Santiago 22, Chile

and

Stefan HOOPS and Heinz SIEDENTOP (*)
Institutt for matematiske fag,
Norges Tekniske Høgskole, N-7034 Trondheim

ABSTRACT. — We show that the excess charge and the ionization energy of the Hellmann-Weizsäcker model of an atom are uniformly bounded in the nuclear charge.

RÉSUMÉ. — Nous démontrons que la charge surplus et l'énergie d'ionisation en modèle Hellmann-Weizsäcker d'un atome sont bornés uniformément dans la charge nucléaire.

1. INTRODUCTION

In recent years the excess charge problem for an atom, *i.e.*, the number of electrons that can be bound in excess of the neutral atom has attracted

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considerable attention (*see*, e.g., Simon [12]). It has been shown to be zero for the Thomas-Fermi model (Lieb and Simon [7]) and the Fermi-Hellmann model [8]. For the Thomas-Fermi-Weizsäcker (TFW) model ([3] and Solovej [14, 13]) and a reduced Hartree-Fock model (Solovej [15]) it has been shown to be positive and universally bounded, *i.e.*, bounded independently of the nuclear charge Z. Here we wish to treat the Hellmann-Weizsäcker model which is an important tool in the proof of the Scott conjecture ([9], [11]) and is of interest in itself. The Hellmann-Weizsäcker model is given through the functional

$$\mathcal{E}_Z^{HW}(\psi) = \sum_{l=0}^{\infty} \int_0^{\infty} \psi_l'(r)^2 + \frac{\alpha_l}{3}\psi_l(r)^6 + \left(\frac{\beta_l}{r^2} - \frac{Z}{r}\right)\psi_l(r)^2\, dr + D\left(\sum_{l=0}^{\infty}\psi_l^2, \sum_{l=0}^{\infty}\psi_l^2\right) \quad (1)$$

with

$$D(f, g) = \frac{1}{2}\int_0^{\infty}\int_0^{\infty}\frac{f(r)g(r')}{\max\{r, r'\}}\, dr\, dr'$$

where ψ is in the set

$$W = \left\{\psi \,\middle|\, \psi = (\psi_1, \psi_2, \ldots) \in \bigoplus_{l=0}^{\infty} H_0^1(0, \infty), \sum_{l=0}^{\infty}\beta_l\int_0^{\infty}\frac{\psi_l(r)^2}{r^2}\, dr < \infty, \psi \geqq 0\right\}. \quad (2)$$

The constants α_l, β_l are $\alpha_l = \left(\frac{\pi}{q(2l+1)}\right)^2$, q the number of spinstates per electron, usually $q=2$, and $\beta_1 = l(l+1)$. The function $\psi_l(r)^2$ may be interpreted as the radial density of electrons with the angular momentum square $l(l+1)$, and thus $\rho(r) = \sum_{l=0}^{\infty}\psi_l(r)^2$ as the radial density of electrons.

A certain restriction (finite particle number and finite number of occupied channels l) of this model has been treated in [8]. Here we wish to investigate the absolute minimizer ψ of (1) in (2) and in (2) under a restriction on the particle number $\int_0^{\infty}\rho(r)\, dr$. We write

$$E^{HW}(Z) = \inf\{\mathcal{E}_Z^{HW}(\psi) \mid \psi \in W\}$$

and

$$E^{HW}(Z, N) = \inf\left\{\mathcal{E}_Z^{HW}(\psi) \mid \psi \in W, \int_0^{\infty}\rho(r)\, dr \leqq N\right\}.$$

In Section 2 we give some basic results on the excess charge Q, namely $Q \leqq Z$. To be explicit, let ψ be the minimizer of $\mathscr{E}_Z^{HW}$, *i.e.*,

$$\rho(r) = \sum_{l=0}^{\infty} \psi_l(r)^2$$

is the minimizing density and $\varphi(r) = \frac{Z}{r} - \int_0^\infty \frac{\rho(r')}{\max\{r, r'\}} dr'$ the corresponding electrical potential; $N_c(Z) = \int_0^\infty \rho(r)\, dr$ is called the critical particle number of te model and $Q(Z) = N_c(Z) - Z$ is the excess charge.

Section 3 and 4 give lower and upper bounds on $E^{HW}(Z)$. The basic idea is to separate the space into an inner part of radius R, where the problem is treated exactly, whereas in an outer region, where intuitively the excess charge is sitting, two approximation schemes are used. In this outer region the screened nuclear charge $\nu(r) = Z - \int_0^\infty \rho(r')\, dr'$ only is effective. Finally Section 6 contains the desired universal bound on the excess charge Q and, moreover, a corresponding bound on the ionization energy $I(Z) = E^{HW}(Z, N_c - 1) - E^{HW}(Z))$. These follow from our main result.

THEOREM 1. — *For all* $\delta > 0$ *there exist* α, $D > 0$ *such that for all* r *satisfying*

$$\alpha Z^{-1/3} \leqq r \leqq D \tag{3}$$

we have

$$(324\,\pi^2 - \delta)\, r^{-3} \leqq \nu(r) \leqq (324\,\pi^2 + \delta)\, r^{-3} \tag{24}$$

and

$$(81\,\pi^2 - \delta)\, r^{-4} \leqq \varphi(r) \leqq (81\,\pi^2 + \delta)\, r^{-4}. \tag{5}$$

Our aim is to prove the following result.

THEOREM 2. — *The excess charge* Q(Z) *and the ionization energy* I(Z) *are bounded by universal constants.*

Our strategy is based on a method for controlling the screening of electrons by Fefferman and Seco ([4], [5]) which has been introduced with the above idea of separation of space in the excess charge problems by Solovej [15].

2. BOUNDS ON THE EXCESS CHARGE AND ON THE NUMBER OF OCCUPIED ANGULAR MOMEMTUM CHANNELS

The purpose of this section is to find a bound on the number of occupied angular momentum channels, *i.e.*, a bound on the maximum l for which ψ_l is not identically zero. This fact in turn implies the existence of a minimizer for the Hellmann-Weizsäcker energy functional when no restriction is imposed on the number of angular momentum channels. We start by considering the Hellmann-Weizsäcker functional (1) restricted to a fixed number of angular momentum channels, say L, *i.e.*, we consider

$$\mathscr{E}^{HW}_{Z,L}(\psi) = \sum_{l=0}^{L} \int_0^\infty \psi_l'(r)^2 + \frac{\alpha_l}{3}\psi_l(r)^6 + \left(\frac{\beta_l}{r^2} - \frac{Z}{r}\right)\psi_l(r)^2\, dr + D\left(\sum_{l=0}^{L} \psi_l^2, \sum_{l=0}^{L} \psi_l^2\right) \quad (6)$$

defined on the set

$$W_L = \left\{ \psi \,\middle|\, \psi = (\psi_1, \ldots, \psi_L) \in \bigoplus_{l=0}^{L} H_0^1(0, \infty), \sum_{l=0}^{L} \beta_l \int_0^\infty \frac{\psi_l(r)^2}{r^2} dr < \infty, \psi \geqq 0 \right\} \quad (7)$$

where α_l and β_l are given as in the introduction. This model has been considered in [8], where the existence of a minimizer of $\mathscr{E}^{HW}_{Z,L}(\psi)$ on W_L has been established and many of the properties of the minimizer have been determined. In the particular, the minimizer satisfies the Euler equation

$$-\psi_l''(r) + \alpha_l \psi_l(r)^5 + \left(\frac{\beta_l}{r^2} - \frac{Z}{r} + \int_0^\infty \frac{\rho(r')}{\max\{r, r'\}} dr'\right)\psi_l(r) = 0, \quad (8)$$

for $l = 0, \ldots, L$, where $\rho(r) = \sum_{l=0}^{L} \psi_l(r)^2$.

Now, let $Q = \int_0^\infty \rho(r)\, dr - Z$ be the "excess charge". We have the following result.

LEMMA 1 (Preliminary bound on the excess charge):

$$Q < Z.$$

Remark. – A similar result for the TFW model is well known (*see*, e. g., [6], Theorem 7.23). Here we adapt the proof in [6] to the Hellmann-Weizsäcker model.

Proof. — Multiply (8) by $r\psi_l(r)$ and sum over l from 0 to L. By dropping the explicitly positive terms we get

$$-\sum_{l=0}^{\mathrm{L}}\int_0^\infty r\psi_l''(r)\psi_l(r)\,dr<\mathrm{ZN}_c-\int_0^\infty\int_0^\infty\frac{r\rho(r)\rho(r')}{\max\{r,r'\}}dr\,dr' \qquad (9)$$

where $\mathrm{N}_c=\mathrm{Q}+\mathrm{Z}$. By integration by parts (note that $\psi_l(r)\sim r^{l+1}$ near the origin and ψ_l decays exponentially at infinity [8]) we get

$$-\int_0^\infty r\psi_l''(r)\psi_l(r)\,dr=\int_0^\infty r\psi_l'(r)^2\,dr\geqq 0,\quad \text{for all } l, \qquad (10)$$

and positive for at least one ψ_l. Moreover,

$$\int_0^\infty\int_0^\infty\frac{r\rho(r)\rho(r')}{\max\{r,r'\}}dr\,dr'=\frac{1}{2}\int_0^\infty\int_0^\infty\frac{r+r'}{\max\{r,r'\}}\rho(r)\rho(r')\,dr\,dr'$$
$$\geqq\frac{1}{2}\left(\int_0^\infty\rho(r)\,dr\right)^2=\frac{1}{2}\mathrm{N}_c^2 \qquad (11)$$

Hence, from (9), (10), and (11) we get $\mathrm{N}_c<2\mathrm{Z}$ which proves the lemma. ■

We now prove two technical lemmas which will be used to bound the maximum number of occupied angular momentum channels.

LEMMA 2. — *For* $l=0,1,\ldots,\mathrm{L}$, *the function* $u_l(r)=\psi_l(r)/r^{l+1}$ *is decreasing in* $(0,\infty)$.

Proof. — The function u_l satisfies the equation

$$u_l''(r)+\frac{2(l+1)}{r}u_l'(r)$$
$$=\alpha_l r^{4(l+1)}u_l(r)^5-\frac{\mathrm{Z}}{r}u_l(r)+u_l(r)\int_0^\infty\frac{\rho(r')}{\max\{r,r'\}}dr'. \qquad (12)$$

Moreover, u_l satisfies the Kato cusp condition (*see*, e. g., [6], Theorem 7.25 and references therein):

$$2(l+1)u_l'(0)+\mathrm{Z}u_l(0)=0$$

and therefore $u'_l(0)<0$. The "potential" $\varphi(r)=\frac{\mathrm{Z}}{r}-\int_0^\infty\frac{\rho(r')}{\max\{r,r'\}}dr'$ satisfies $(r\varphi(r))''=\frac{1}{r}\rho(r)$ for $r\neq 0$, *i.e.*, $r\varphi(r)$ is convex and it has a unique zero R_0, [8]. For $r<\mathrm{R}_0$ we have $\varphi(r)>0$. Using $\varphi(r)$ equation (12) reads

$$u_l''(r)+\frac{2(l+1)}{r}u_l'(r)=\alpha_l r^{4(l+1)}u_l(r)^5-\varphi(r)u_l(r). \qquad (13)$$

From this equation it is clear that the only critical points of u_l for $r \geqq R_0$ are minima. Since u_l goes to zero at infinity, it follows that $u_l'(r)<0$ for all $r \geqq R_0$. To finish the proof, assume u_l is not necessarily decreasing in $(0, R_0)$. Then, using (13), there exist two points $r_1 < r_2$ such that $u_l'(r_1) = u_l'(r_2) = 0$, $u_l(r_1) < u_l(r_2)$ and $u_l''(r_1) > 0 > u_l''(r_2)$. From (13), and the fact that $r\varphi(r)$ is decreasing in $(0, R_0)$ we get

$$0 < \frac{u_l''(r_1)}{u_l(r_1)} = \alpha_l r_1^{4(l+1)} u_l(r_1)^4 - \varphi(r_1)$$

$$< \alpha_l r_2^{4(l+1)} u_l(r_2)^4 - \varphi(r_2) = \frac{u_l''(r_2)}{u_l(r_2)} < 0,$$

which proves the lemma. ■

Remark. — The proof of this lemma is patterned after the proof of [6], Theorem 7.26.

We have the following result.

LEMMA 3. — *For all* $l = 0, 1, \ldots, L$

$$\psi_l(r)^2 \leqq \frac{2l+3}{r} N_l, \qquad \textit{with} \quad N_l = \int_0^\infty \psi_l(r)^2 \, dr.$$

Proof. — Since u_l is decreasing,

$$\int_0^\infty \psi_l(r)^2 \, dr \geqq \int_0^r t^{2(l+1)} u_l(t)^2 \, dt \geqq u_l(r)^2 \frac{r^{2l+3}}{2l+3} = \frac{r}{2l+3} \psi_l(r)^2. \quad ■$$

With all these preliminary results we can find a bound on the maximum l, say l_c, having a nontrivial ψ_l, *i.e.*, a bound on the number of occupied angular momentum channels. This in turn implies the existence of a minimizer for the unrestricted Hellmann-Weizsäcker energy functional.

THEOREM 3. — *Consider the restricted Hellmann-Weizsäcker minimization problem* (6), (7), *and* l_c *defined as above. Then*

$$l_c \leqq \sqrt{\frac{24 Z}{q}}. \tag{14}$$

Proof. — Let $N_l = \int_0^\infty \psi_l(r)^2 \, dr$ be as above. We first prove that for the minimizing ψ,

$$N_l \geqq \frac{2l+1}{2l+3} \frac{q}{\pi} \sqrt{l_c(l_c+1) - l(l+1)},$$

for all $l = 0, 1, \ldots, l_c - 1$. Let us assume, in the contrary, that

$$N_l < \frac{2l+1}{2l+3} \frac{q}{\pi} \sqrt{l_c(l_c+1) - l(l+1)}$$

for some $0 \leqq l < l_c$. Then choose the trial function $\tilde{\psi} = (\tilde{\psi}_1, \tilde{\psi}_2, \ldots, \tilde{\psi}_L)$ with $\tilde{\psi}_{l'} = \psi_l$ for $l' \neq l$, $l' \neq l_c$ and $\tilde{\psi}_l^2 = \psi_l^2 + \varepsilon \psi_{l_c}^2$, $\tilde{\psi}_{l_c}^2 = (1-\varepsilon)\psi_{l_c}^2$. Here $\varepsilon > 0$ is small and obviously $\tilde{\rho} = \rho$. By using the subadditivity of the kinetic energy term (*see*, e. g., [2]).

$$\int_0^\infty \tilde{\psi}_l'(r)^2\, dr \leqq \int_0^\infty \psi_l'(r)^2\, dr + \varepsilon \int_0^\infty \psi_{l_c}'(r)^2\, dr$$

and therefore, if we denote $\tilde{\mathscr{E}} = \mathscr{E}_{Z,L}^{HW}(\tilde{\psi}_l)$ and $\mathscr{E} = \mathscr{E}_{Z,L}^{HW}(\psi_l)$, we have, to first order in ε

$$\tilde{\mathscr{E}} - \mathscr{E} = \varepsilon \int_0^\infty \psi_{l_c}(r)^2 \left(\alpha_l \psi_l(r)^4 - \alpha_{l_c} \psi_{l_c}(r)^4 + \frac{\beta_l}{r^2} - \frac{\beta_{l_c}}{r^2} \right) dr + O(\varepsilon^2).$$

Dropping the negative $-\alpha_{l_c} \psi_{l_c}(r)^4$ and using Lemma 3 we get

$$\tilde{\mathscr{E}} - \mathscr{E}$$
$$\leqq \varepsilon \int_0^\infty \psi_{l_c}(r)^2 \left(\alpha_l \frac{(2l+3)^2}{r^2} N_l^2 + \frac{l(l+1)}{r^2} - \frac{l_c(l_c+1)}{r^2} \right) dr + \text{Const}\, \varepsilon^2 < 0$$

because of the choice of N_l. But this contradicts for sufficiently small but positive ε the fact that ψ is the minimizer of $\mathscr{E}_{Z,L}^{HW}$. Thus

$$N_l > \frac{2l+1}{2l+3} \frac{q}{\pi} \sqrt{l_c(l_c+1) - l(l+1)} > \frac{q}{3\pi} \sqrt{l_c(l_c+1) - l(l+1)}$$

for all $0 \leqq l < l_c$. However, from Lemma 1 we have

$$2Z > \sum_{l=0}^{l_c} N_l > \sum_{l=0}^{l_c - 1} N_l > \frac{q}{3\pi} \sum_{l=0}^{l_c - 1} \sqrt{l_c(l_c+1) - l(l+1)}.$$

The right side of this equation can be bounded from below by

$$\frac{q}{3\pi} \int_0^{l_c} \sqrt{l_c^2 - x^2}\, dx = \frac{q}{3\pi} l_c^2 \frac{\pi}{4},$$

and this concludes the proof of the theorem. ■

Remark. — The bound (14) is not optimal. We believe the best bound should be proportional to $Z^{1/3}$ as in the Bohr model or the Fermi-Hellmann model [1].

3. LOWER BOUND

Given $R>0$ and $0<s<\frac{1}{4}R$ pick two C^∞-functions $\theta_\pm:(0,\infty)\to[0,\infty)$ such that $\theta_+^2+\theta_-^2=1$ and

$$\theta_+(r)=\begin{cases}0 & r\leqq R-s\\ 1 & r\geqq R+s\end{cases} \quad \text{and} \quad |\theta'\pm(r)|\leqq c_\theta s^{-1}. \tag{15}$$

Again let ψ be the absolute minimizer of $\mathcal{E}_Z^{HW}$. An IMS formula for the case at hand reads

$$\sum_{l=0}^\infty \int_0^\infty \psi_l'(r)^2\,dr=\sum_{l=0}^\infty \int_0^\infty (\theta_+\psi_l)'(r)^2+(\theta_-\psi_l)'(r)^2\,dr - \sum_{l=0}^\infty \int_0^\infty \psi_l(r)^2(\theta_+'(r)^2+\theta_-'(r)^2)\,dr.$$

For technical purpose we define

$$\bar{\nu}=Z-\int_0^\infty \theta_-(r)^2\rho(r)\,dr$$

which gives rise to a screened outer Fermi-Hellmann functional

$$\mathcal{E}^H_{\bar{\nu},R-s}(\underline{\rho})=\sum_{l=0}^\infty \int_{R-s}^\infty \frac{\alpha_l}{3}\rho_l(r)^3+\left(\frac{(l+1/2)^2}{r^2}-\frac{\bar{\nu}}{r}\right)\rho_l(r)\,dr + 2D\left(\sum_{l=0}^\infty \rho_l,\rho^{TF}_{\bar{\nu},R-s}\right)-D(\rho^{TF}_{\bar{\nu},R-s},\rho^{TF}_{\bar{\nu},R-s})$$

where $\rho^{TF}_{\bar{\nu}R-s}$ is the solution of the outer Thomas-Fermi minimization problem (Solovej [15]). Analogously define

$$\varphi^{TF}_{\bar{\nu},R-s}(r)=\frac{\bar{\nu}}{r}-\int_0^\infty \frac{\rho^{TF}_{\bar{\nu},R-s}(r')}{\max\{r,r'\}}\,dr.$$

Moreover it is easy to check (Solovej [15]) that

$$\int_0^\infty \int_0^\infty \frac{\theta_-(r)^2\rho(r')}{\max\{r,r'\}}\,dr'-\frac{Z-\bar{\nu}}{r}\theta_+(r)^2\rho(r)\,dr = -\int_{R-s}^{R+s}\int_r^{R+s}\left(\frac{1}{r}-\frac{1}{r'}\right)\theta_+(r)^2\rho(r)\theta_-(r')^2\rho(r')\,dr'\,dr\leqq 0.$$

Thus using Hardy's inequality

$$E^{HW}(Z)\geqq \mathcal{E}_Z^{HW}(\theta_-\psi)+\mathcal{E}^H_{\bar{\nu},R-s}(\theta_+^2\psi^2)+D(\theta_+^2\rho-\rho^{TF}_{\bar{\nu}R-s},\theta_+^2\rho-\rho^{TF}_{\bar{\nu},R-s}) - \int_{R-s}^{R+s}(\theta_-'(r)^2+\theta_+'(r)^2)\rho(r)\,dr$$

$$-\int_{R-s}^{R+s}\int_{r}^{R+s}\left(\frac{1}{r}-\frac{1}{r'}\right)\theta_+(r)^2\rho(r)\,\theta_-(r')^2\rho(r')\,dr'\,dr.$$

Because of condition (15) and writing $Q_\Delta(R, s)=\int_{R-s}^{R+s}\rho(r)\,dr$ we obtain

$$\int_{R-s}^{R+s}(\theta'_+(r)^2+\theta'_-(r)^2)\,\rho(r)\,dr\leqq 2\,c_\theta\,s^{-2}\,Q_\Delta(R, s)$$

for the next to last summand. The last summand is bounded by $2s/(R^2-s^2)\,Q_\Delta(R, s)^2$. Denoting the absolute minimum of $\mathscr{E}^H_{\bar{v}, R-s}$ by $E^H_{R-s}(\bar{v})$ we have the following

$$E^{HW}(Z)\geqq\mathscr{E}^{HW}_Z(\theta_-\psi)+E^H_{R-s}(\bar{v})+D(\theta_+^2\,\rho-\rho^{TF}_{\bar{v}, R-s},\,\theta_+^2\,\rho-\rho^{TF}_{\bar{v}, R-s})$$
$$-2\,c_\theta\,s^{-2}\,Q_\Delta(R, s)^2-2\frac{s}{R^2-s^2}\,Q_\Delta(R, s)^2. \quad (16)$$

For further use we denote the minimizer of $\mathscr{E}^H_{\bar{v}, R-s}$ by ρ^H, explicitly

$$\rho^H_l(r)=\alpha_l^{-1/2}\left[\varphi^{TF}_{\bar{v}, R-s}(r)-\frac{(l+1/2)^2}{r^2}\right]_+^{1/2}\qquad\text{for}\quad r\geqq R-s$$

and $\rho^H(r)=\sum_{l=0}^{\infty}\rho^H_l(r)$.

4. UPPER BOUND

Since we are dealing with a minimization problem, it suffices to pick a set of trial functions. Let $r_2(l)$ be the largest point in the support of ρ^H_l (see also Definition 2.1 in [9]). According to Appendix A (proof of Lemma 6) we can use the bound

$$\frac{3\pi}{2q(2l+1)}\sqrt{x_m^3\,\varphi^{TF}(x_m)}\leqq r_2(l)\leqq\frac{36\pi}{q(2l+1)}$$

([9], Proposition 4.1, formula 2) where x_m denotes the maximum of $r^2\,\varphi^{TF}(r)$ which is of order $Z^{-1/3}$. Due to Lemma 6 we can always assume that $R+s\geqq x_m$, if we take $\alpha Z^{-1/3}\leqq R$. Define $x_2(l)=r_2(l)-SZ^{-2/3}$ with a positive constant S to be chosen later. We choose the trial function

$$f_l(r)=\begin{cases}\theta_-(r)\,\psi_l(r) & r\leqq R+s\\ \sqrt{\tilde{\rho}_l(r)} & r\geqq R+s.\end{cases}$$

In the case $R+2s \geqq x_2(l)$ we take $\tilde{\rho}_l(r)=0$. In the other case $R+2s<x_2(l)$ we choose

$$\tilde{\rho}_l(r)=\begin{cases} 0 & r \leqq R+s \\ s^{-2}\rho_l^H(R+2s)(r-(R+s))^2 & R+s \leqq r \leqq R+2s \\ \rho_l^H(r) & R+2s \leqq r \leqq x_2(l) \\ \tilde{\beta}_l^2 e^{-2\gamma r} & x_2(l) \leqq r \end{cases}$$

where $\tilde{\beta}_l^2=\rho_l^H(x_2(l))e^{2\gamma x_2(l)}$ and $\gamma=\bar{v}^{2/3}$. Note that $\underline{f}=(f_1, f_2, \ldots)$ is in W. This yields

$$\begin{aligned} E^{HW}(Z) &\leqq \mathscr{E}_Z^{HW}(\theta_-\psi)+\mathscr{E}_{Z,0}^{HW}(\underline{\tilde{\rho}})+D(\tilde{\rho}-\rho_{\bar{v},R-s}^{TF}, \tilde{\rho}-\rho_{\bar{v},R-s}^{TF}) \\ &\quad +\sum_{l=0}^{\infty}\int_0^{\infty}\theta_-(r)^2\psi_l(r)^2\,dr\int_0^{\infty}\frac{\tilde{\rho}_{l'}(r')}{r'}\,dr' \\ &\quad +\sum_{l=0}^{\infty}\int_0^{\infty}\tilde{\rho}_l^{1/2'}(r)^2-\frac{1}{4r^2}\tilde{\rho}_l(r)\,dr \\ &\leqq \mathscr{E}_Z^{HW}(\theta_-\psi)+\mathscr{E}_{\bar{v},R+s}^{H}(\underline{\tilde{\rho}})+D(\tilde{\rho}-\rho_{\bar{v},R-s}^{TF}, \tilde{\rho}-\rho_{\bar{v},R-s}^{TF}) \\ &\quad +\sum_{l=0}^{\infty}\int_0^{\infty}\tilde{\rho}_l^{1/2'}(r)^2\,dr \end{aligned}$$

where $\tilde{\rho}(r)=\sum_{l=0}^{\infty}\tilde{\rho}_l(r)$. We wish to estimate the last three terms by $\mathscr{E}_{\bar{v},R-s}^{H}(\chi_{[R+s,\infty)}\underline{\rho}^H)$ plus a small remainder.

First case $(R+2s \geqq x_2(l))$: Here it suffices to bound $\sum_{l=0}^{\infty}\int_{R+s}^{r_2(l)}\frac{\bar{v}}{r}\rho_l^H(r)\,dr$, where the sum is only taken over l which fulfill $x_2(l)\leqq R+2s\leqq r_2(l)$, which according to (23) is $O\left(\frac{\bar{v}^{4/3}}{(R+s)^2}\right)$ because the constraint allows for finitely many l uniformly in $\bar{v}$ and $\text{const}\,\bar{v}^{1/3}\leqq l\leqq \text{Const}\,\bar{v}^{1/3}$.

Second case $(R+2s<x_2(l))$: Since

$$\sum_{l=0}^{\infty}\int_{x_2(l)}^{\infty}f_l'(r)^2+\frac{\alpha}{3}f_l(r)^6+\frac{(l+1/2)^2}{r^2}f_l(r)^2\,dr = \sum_{l=0}^{c\bar{v}^{1/3}}O\left(\bar{v}^{7/6}\left(l+\frac{1}{2}\right)\right)=O(\bar{v}^{11/6})$$

([9], (3.4)). We also used $l\leqq \text{Const}\,\bar{v}^{1/3}$. Moreover

$$\sum_{l=0}^{\infty}\int_0^{\infty}\int_0^{\infty}\frac{f_l(r)^2\rho_{\bar{v},R-s}^{TF}(r')}{\max\{r,r'\}}\leqq 2D(\rho^H, \rho_{\bar{v},R-s}^{TF})+O(\bar{v}^2),$$

since f_l^2 is dominated by ρ^H left of $R+2s$ and inequality (24). Also

$$\sum_{l=0}^{\infty} \int_{R+s}^{x_2(l)} f_l'(r)^2\, dr = \sum_{l=0}^{\infty} \left(\frac{\rho_l^H(R+2s)}{s} + \int_{R+2s}^{x_2(l)} f_l'(r)^2\, dr \right)$$
$$= \sum_{l=0}^{c\bar{\nu}^{1/3}} O\left(l \left(\frac{c}{(R+2s)^4} - \frac{l^2}{(R+s)^2} \right)^{-1/2} + \frac{\bar{\nu}^{1/3}}{\min\{l+1/2, \bar{\nu}^{1/4}\}(l+1/2)^{1/2}} \right)$$
$$= O\left(\frac{1}{s(R+2s)^{5/2}} \right) + O(\bar{\nu}^{37/24}).$$

For the second equality (second summand) *see* [9], (3.9). Finally, by (25),

$$D(\tilde{\rho} - \rho_{\bar{\nu}, R-s}^{TF}, \tilde{\rho} - \rho_{\bar{\nu}, R-s}^{TF}) \leqq O\left(\frac{1}{R^{17/3}} + \frac{\bar{\nu}}{R^{7/3}} + \bar{\nu}^{5/3} \right).$$

Thus

$$E^{HW}(Z) \leqq \mathcal{E}_Z^{HW}(\theta - \psi) + \mathcal{E}_{\bar{\nu}, R-s}^{H}(\chi_{[R+s, \infty)}\, \underline{\rho}^H)$$
$$+ O\left(\frac{1}{s(R+2s)^{5/2}} + \bar{\nu}^2 + \frac{1}{R^{17/3}} + \frac{\bar{\nu}}{R^{7/3}} + \bar{\nu}^{5/3} + \frac{\bar{\nu}^{4/3}}{(R+s)^2} \right).$$

Dropping the characteristic function in the argument of $\mathcal{E}_{\bar{\nu}, R-s}^{H}$ generates an error which is bounded by $\int_{R-s}^{R+s} \frac{\bar{\nu}}{r} \rho^H(r)\, dr = O\left(\bar{\nu}^{5/3} \frac{R_s}{(R^2 - s^2)^2} \right)$ yielding the bound

$$E^{HW}(Z) \leqq \mathcal{E}_Z^{HW}(\theta_- \psi) + \mathcal{E}_{\bar{\nu}, R-s}^{H}(\underline{\rho}^H)$$
$$+ O\left(\frac{1}{s(R+2s)^{5/2}} + \bar{\nu}^2 + \frac{1}{R^{17/3}} + \frac{\bar{\nu}}{R^{7/3}} + \frac{\bar{\nu}^{5/3} R s}{(R^2 - s^2)^2} + \frac{\bar{\nu}^{4/3}}{(R+s)^2} \right).$$

Combining upper and lower bound gives the following estimate

$$D(\theta_+^2 \rho - \rho_{\bar{\nu}, R-s}^{TF}, \theta_+^2 \rho - \rho_{\bar{\nu}, R-s}^{TF})$$
$$\leqq 2 c_\theta s^{-2} Q_\Delta(R, s) + 2 \frac{s}{R^2 - s^2} Q_\Delta(R, s)^2$$
$$+ O\left(\frac{1}{s(R+2s)^{5/2}} + \bar{\nu}^2 + \frac{1}{R^{17/3}} + \frac{\bar{\nu}}{R^{7/3}} + \bar{\nu}^{5/3} \frac{R_s}{(R^2 - s^2)^2} + \frac{\bar{\nu}^{4/3}}{(R+s)^2} \right). \quad (17)$$

For $R = s = 0$ the following holds

$$E^{TF}(Z, Z) - c Z^{5/3} + D(\rho - \rho_{\bar{\nu}, R-s}^{TF}, \rho - \rho_{\bar{\nu}, R-s}^{TF})$$
$$\leqq \sum_{l=0}^{\infty} \int_0^{\infty} \psi_l'(r)^2 + \frac{\alpha_l}{3} \psi_l(r)^6 + \left(\frac{l(l+1)}{r^2} - \varphi^{TF}(r) \right) \psi_l(r)^2\, dr$$
$$- D(\rho_{\bar{\nu}, R-s}^{TF}, \rho_{\bar{\nu}, R-s}^{TF}) - c Z^{5/3} + D(\rho - \rho_{\bar{\nu}, R-s}^{TF}, \rho - \rho_{\bar{\nu}, R-s}^{TF})$$
$$= E^{HW}(Z) \leqq E^{TF}(Z, Z) + O(Z^{(7/3)(1-\varepsilon)}) \quad (18)$$

for all $0 \leqq \varepsilon \leqq \frac{1}{7}$. The first inequality follows from Poisson summation ([9] and also [10], p. 191, first inequality), Hardy's inequality, and the explicit solution of the Fermi-Hellmann equation for external potential φ^{TF}; the second inequality follows from the estimates (3.4-11) of [9].

5. SUCCESSIVE SCREENING OF THE NUCLEAR CHARGE

The purpose of this section is to show that the separation of space at radius R may be pushed from $R=0$ to unit distance (on scale $Z^{-1/3}$) thus yielding error terms independent of Z. First we can transcribe Lemma 6 of Solovej [15].

LEMMA 4. – *There exist constants* α, $\beta \geqq 0$ *such that for*

$$\alpha Z^{-1/3} < R \leqq \beta Z^{-(1/3)(1-\varepsilon)}$$

we have inequalities (4) *and* (5).

Proof. – The proof is analogue to Solovej's result and uses inequality (18). ■

Next we come to the heart of successive screening.

LEMMA 5. – *Given* $\delta > 0$ *there exists* $D_1(\delta) > 0$ *such that, if* (4) *and* (5) *hold for* r *and* Z *satisfying*

$$a := \alpha Z^{-1/3} < r \leqq \beta Z^{-(1/3)(1-\varepsilon)^n} =: b_n \leqq D_1(\delta) \tag{19}$$

with α, β *as in Lemma* 4, *and* $n \in \mathbb{N}$, *then* (4) *and* (5) *hold for*

$$a < r \leqq b_{n+1}$$

Proof. – First we follow [15]. We assume that Z satisfy (19) implies (4) and (5). Note that

$$\frac{4}{3} a < \frac{4}{5} b_1 \qquad \text{if} \quad D_1(\delta) < \frac{3}{5} \beta^{1/\varepsilon} \alpha^{1-1/\varepsilon}.$$

Now for $R \in \left(\frac{4}{3} a, \frac{4}{5} b_n\right)$ pick $s = R^{\eta+1}$, where we choose η such that $\left(\frac{4}{5} D_1(\delta)\right)^\eta \leqq \frac{1}{4}$ implies $s \leqq \frac{R}{4}$. For $\theta_\pm$ as in Section 3 we have (4), since $R-s$ and $R+s$ satisfy (19). Thus, since $\nu(R+s) \leqq \bar{\nu} \leqq \nu(R-s)$, we obtain

$$(324\pi^2 - \delta)\left(\frac{4}{5}\right)^3 R^{-3} \leqq \bar{\nu} \leqq (324\pi^2 + \delta)\left(\frac{4}{3}\right)^3 R^{-3}.$$

This gives

$$Q_\Delta(R, s)=\nu(R-s)-\nu(R+s)$$
$$\leqq\left[(324\pi^2+\delta)\left(\frac{4}{3}\right)^3-(324\pi^2-\delta)\left(\frac{4}{5}\right)^3\right]R^{-3}=c'_\delta R^{-3}.$$

In particular

$$\bar{\nu}(R-s)^3\geqq\bar{\nu}\left(\frac{3}{4}\right)^3 R^3\geqq(324\pi^2-\delta)\left(\frac{3}{5}\right)^3. \tag{20}$$

From (17) we obtain

$$D(\theta_+^2\rho-\rho^{TF}_{\bar{\nu}, R-s}, \theta_+^2\rho-\rho^{TF}_{\bar{\nu}, R-s})$$
$$\leqq O(s^{-2}R^{-3}+sR^{-8}+R^{-6})=O(R^{-19/3})\leqq c_\delta D_1(\delta)^{1/3}R^{-7(1-\varepsilon)} \tag{21}$$

where we pick $\eta=\dfrac{2}{3}$ and where $\varepsilon=\dfrac{1}{21}$ (which is covered by the hypothesis of (18)) and use $R\leqq D_1(\delta)<1$.

By (20) and [15], (4.13), we can find $\tilde{\alpha}(\delta)>0$ such that for $\tilde{R}\geqq\dfrac{3}{4}\tilde{\alpha}(\delta)R$

$$\left(324\pi^2-\frac{\delta}{2}\right)\tilde{R}^{-3}\leqq\int_{\tilde{R}}^{\infty}\rho^{TF}_{\bar{\nu}, R-s}(r)\,dr\leqq\left(324\pi^2+\frac{\delta}{2}\right)\tilde{R}^{-3}.$$

Repeating the argument of Lemma 4 yields for $r\geqq\tilde{\alpha}(\delta)R$

$$-c''_\delta r^{1/2}R^{-(7/2)(1-\varepsilon)}+(324\pi^2-\frac{3}{4}\delta)r^{-3}$$
$$\leqq\bar{\nu}-\int_0^r\theta_+(r')^2\rho(r')\,dr'\leqq c''_\delta r^{1/2}R^{-(7/2)(1-\varepsilon)}+\left(324\pi^2+\frac{3}{4}\delta\right)r^{-3}.$$

Notice

$$\bar{\nu}-\int_0^r\theta_+(r')^2\rho(r')\,dr'=\nu(r)\qquad\text{for}\quad\tilde{\alpha}(\delta)\geqq\frac{5}{4}.$$

For $\tilde{\alpha}(\delta)R\leqq r\leqq\beta_1 R^{(1-\varepsilon)}$ and $\beta_1>0$ we have

$$\left(-c''_\delta D_1(\delta)^{1/6}\beta_1^{-7/2}-\frac{3}{4}\delta+324\pi^2\right)r^{-3}$$
$$\leqq\nu(r)\leqq\left(c''_\delta D_1(\delta)^{1/6}\beta_1^{-7/2}+\frac{3}{4}\delta+324\pi^2\right)r^{-3}.$$

The remaining part of the proof follows as in [15], Lemma 7. ■

Proof of Theorem 1. — Lemma 4 starts the induction and Lemma 5 is the inductive step for the proof of the claimed result for ν. The proof for φ is analogue. ■

6. UNIVERSAL BOUNDS ON THE EXCESS CHARGE AND THE IONIZATION ENERGY

First note that $Q(Z) \leqq Z$ by Lemma 1. Moreover,

$$I(Z) \leqq -E^{HW}(Z) = O(Z^{7/3}).$$

The proof of Theorem 2 follows now by a modification of Lemma 1 for a suitable outside problem.

Proof of Theorem 2. – Fix $R < \frac{1}{4} D$. Pick $I \in C^\infty(\mathbb{R}^3)$ with

$$I(r) = \begin{cases} 0 & r \leqq R \\ 1 & r \geqq 2R \end{cases}$$

where $|I'| \leqq \text{Const.}/R$ and $|I''| \leqq \text{Const.}/R^2$. We have

$$0 = \sum_{l=0}^{\infty} \left(\psi_l, r I(r) \left(-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + \alpha_l \psi_l(r)^4 - \varphi(r) \right) \psi_l \right)$$

$$= \sum_{l=0}^{\infty} \left\{ -(\psi_l, r I(r) \psi_l'') + \int_0^\infty \psi_l(r)^2 r I(r) \left(\frac{l(l+1)}{r^2} + \alpha_l \psi_l(r)^4 - \varphi(r) \right) dr \right\}$$

$$\geqq -\frac{c}{R} \int_R^\infty \rho(r)\, dr - Z \int_0^\infty I(r) \rho(r)\, dr + \int_0^\infty \int_0^\infty r I(r) \frac{\rho(r) \rho(r')}{\max\{r, r'\}} dr\, dr'.$$

We can write

$$\int_0^\infty \int_0^\infty r I(r) \frac{\rho(r)\rho(r')}{\max\{r, r'\}} dr\, dr'$$

$$= \int_0^\infty \int_0^\infty r \frac{I(r)\rho(r) I(r')\rho(r')}{\max\{r, r'\}} dr\, dr' + \int_0^\infty \int_0^\infty r \frac{I(r)\rho(r)(1 - I(r'))\rho(r')}{\max\{r, r'\}} dr\, dr'$$

$$\geqq \frac{1}{2} \int_0^\infty \int_0^\infty (r + r') \frac{I(r)\rho(r) I(r')\rho(r')}{\max\{r, r'\}} dr\, dr' + \int_0^\infty I(r)\rho(r)\, dr \int_0^\infty (1 - I(r'))\rho(r')\, dr' - \frac{1}{2} \left(\int_R^{2R} \rho(r)\, dr \right)^2$$

$$\geqq \frac{1}{2} \left(\int_0^\infty I(r)\rho(r)\, dr \right)^2 + (Z - \nu(2R)) \int_0^\infty I(r)\rho(r)\, dr - \frac{1}{2} \left(\int_R^{2R} \rho(r)\, dr \right)^2.$$

By Theorem 1 we have $\int_{R}^{2R} \rho(r)\,dr < c'$. Thus

$$0 \geqq -\frac{c}{R}\left(\int_0^\infty I(r)\,\rho(r)\,dr + c'\right) - \nu(2R)\int_0^\infty I(r)\,\rho(r)\,dr + \frac{1}{2}\left(\int_0^\infty I(r)\,\rho(r)\,dr\right)^2 - \frac{1}{2}c'^2.$$

Since R and $\nu(R)$ are bounded

$$\int_0^\infty I(r)\,\rho(r)\,dr \leqq \text{Const.}$$

Then we get for the excess charge

$$\begin{aligned} Q(Z) = N_c(Z) - Z = \int_0^\infty \rho(r)\,dr - Z \\ \leqq \int_0^{2R} \rho(r)\,dr - Z + \int_0^\infty I(r)\,\rho(r)\,dr \\ \leqq -\nu(2R) + \text{Const.} \leqq \text{Const.} \end{aligned}$$

To proof the bound for the ionization energy we go back to (16). We can choose R and s so that $\int_0^\infty \theta_-(r)^2\,\rho(r)\,dr \leqq N_c(Z) - 1$. Then we get

$$\mathscr{E}_Z^{HW}(\theta_-\psi) \geqq E^{HW}(Z, N_c(Z) - 1).$$

Thus it suffices to estimate $\mathscr{E}_Z^{HW}(\theta_-\psi) - E^{HW}(Z)$ from above by a constant. Using inequality (16) we have to show

$$\begin{aligned} -E^{H}_{R-s}(\bar{\nu}) - D(\theta_+^2\rho - \rho^{TF}_{\bar{\nu}, R-s}, \theta_+^2\rho - \rho^{TF}_{\bar{\nu}, R-s}) \\ + 2c_\theta s^{-2} Q_\Delta(R, s) + 2\frac{s}{R^2 - s^2} Q_\Delta(R, s) \leqq \text{Const.} \end{aligned} \quad (22)$$

Since $\bar{\nu}$, R and s are bounded by constants and also

$$\begin{aligned} \int_0^\infty \theta_+(r)^2\,\rho(r)\,dr = N_c(Z) - \int_0^\infty \theta_-(r)^2\,\rho(r)\,dr \\ = Q(Z) + \bar{\nu} \leqq \text{Const.}, \end{aligned}$$

we easily see that the inequality (22) holds. Therefore the ionization energy is smaller than a constant. ■

APPENDIX

A. BASIC PROPERTIES OF THE OUTER HELLMANN DENSITY

We want to estimate the maximum of the density ρ_l^{H} which minimize the outer Hellmann functional $\mathscr{E}^{\mathrm{H}}_{\nu,\mathrm{R}}$. The derivative is

$$\frac{d}{dr}\rho_l^{\mathrm{H}}(r) = -\frac{1}{r^2}\left[r^2\varphi^{\mathrm{TF}}_{\nu,\mathrm{R}-s}(r) - \left(l+\frac{1}{2}\right)\right]_+^{1/2} + \frac{1}{2r}\left[r^2\varphi^{\mathrm{TF}}_{\nu,\mathrm{R}}(r) - \left(l+\frac{1}{2}\right)\right]_+^{-1/2}\frac{d}{dr}(r^2\varphi^{\mathrm{TF}}_{\nu,\mathrm{R}}(r)).$$

Therefore the maximum of ρ_l^{H} is left of the maximum of $r^2\varphi^{\mathrm{TF}}_{\nu,\mathrm{R}}(r)$. We compare $\varphi^{\mathrm{TF}}_{\nu,\mathrm{R}}$ and φ^{TF}. Because both functions satisfy the same differential equation we have to look at the boundary conditions. We have $\frac{d}{dr}\varphi^{\mathrm{TF}}_{\nu,\mathrm{R}}(\mathrm{R}) = -\frac{\nu}{\mathrm{R}^2}$ and can calculate

$$\frac{d}{dr}\varphi^{\mathrm{TF}}(\mathrm{R}) = -\frac{1}{\mathrm{R}^2}\left(\mathrm{Z}^{\mathrm{TF}} - \int_0^{\mathrm{R}}\rho^{\mathrm{TF}}(r)\,dr\right),$$

which implies that, for $\nu = \mathrm{Z}^{\mathrm{TF}} - \int_0^{\mathrm{R}}\rho^{\mathrm{TF}}(r)\,dr$, we have the same potentials for $r \geqq \mathrm{R}$. Due to the scaling property of φ^{TF} we get that the maximum $r^2\varphi^{\mathrm{TF}}_{\nu,\mathrm{R}}$ is at $\alpha_m \mathrm{Z}^{-1/3}$ ([9], Appendix). The screened charge ν is of order Z and also of order Z^{TF}. Therefore we have $\mathrm{Z}^{\mathrm{TF}} = O(\mathrm{Z})$. Thus we can use the results of [9] and have proven the following lemma.

LEMMA 6. — *We can choose* $\alpha > 0$ *so that for all* R *satisfying* $\alpha \mathrm{Z}^{-1/3} < \mathrm{R} \leqq \mathrm{Const.}$ *the density* ρ_l^{H} *has no maximum for* $r \geqq \mathrm{R}$.

B. ESTIMATE OF INTEGRALS

We have

$$\int_{\mathrm{R}+s}^{r_2(l)} \frac{\bar{\nu}}{r}\rho_l^{\mathrm{H}}(r)\,dr = \bar{\nu}\int_{\mathrm{R}+s}^{\infty} \frac{2q}{\pi r^2}\left(l+\frac{1}{2}\right)\left[r^2\varphi^{\mathrm{TF}}_{\nu,\mathrm{R}-s}(r) - \left(l+\frac{1}{2}\right)^2\right]_+^{1/2} dr$$
$$\leqq \mathrm{Const.}\, l\bar{\nu}\int_{\mathrm{R}+s}^{\infty}\frac{1}{r^3}\,dr \leqq \mathrm{Const.}\frac{l\bar{\nu}}{(\mathrm{R}+s)^2} \tag{23}$$

where the first inequality follows from [15], Theorem 3.3, for $R+s$ big enough. Furthermore

$$\sum_{l=0}^{\infty}\int_0^{\infty}\int_0^{\infty}\frac{f_l(r)^2\,\rho^{TF}_{\bar{v},R-s}(r')}{\max\{r,r'\}}\,dr\,dr' \leqq \sum_{l=0}^{\infty}\int_0^{\infty}\int_0^{\infty}\frac{\rho^{H}_l(r)\,\rho^{TF}_{\bar{v},R-s}(r')}{\max\{r,r'\}}\,dr\,dr' + \sum_{l=0}^{\infty}\int_0^{\infty}\int_{x_2(l)}^{\infty}\frac{\beta^2 e^{-2\gamma r}\,\rho^{TF}_{\bar{v},R-s}}{\max\{r,r'\}}\,dr\,dr'$$

where

$$\sum_{l=0}^{\infty}\int_0^{\infty}\int_{x_2(l)}^{\infty}\frac{\beta^2 e^{-2\gamma r}\,\rho^{TF}_{\bar{v},R-s}(r')}{\max\{r,r'\}}\,dr\,dr' \leqq \text{Const.}\,\bar{v}^{1/3}\sum_{l=0}^{\infty}\frac{1}{x_2(l)}\rho^{H}_l(x_2(l))$$

$$\leqq \text{Const.}\,\bar{v}^{1/3}\sum_{l=0}^{c\bar{v}^{1/3}}\left(l+\frac{1}{2}\right)\frac{1}{x_2(l)}\left[\varphi^{TF}_{\bar{v},R-s}(x_2(l))-\frac{(l+1/2)^2}{x_2(l)^2}\right]_+^{1/2}$$

$$\leqq \text{Const.}\,\bar{v}^{1/3}\sum_{l=0}^{c\bar{v}^{1/3}}\frac{l}{x_2(l)^3}\leqq \text{Const.}\,\bar{v}^{1/3}\sum_{l=0}^{c\bar{v}^{1/3}} l^4 = O(\bar{v}^2).$$

Putting this result and the previous inequality together yields the desired bound

$$\sum_{l=0}^{\infty}\int_0^{\infty}\int_0^{\infty}\frac{f_l(r)^2\,\rho^{TF}_{\bar{v},R-s}(r')}{\max\{r,r'\}}\,dr\,dr' \leqq \sum_{l=0}^{\infty}\int_0^{\infty}\int_0^{\infty}\frac{\rho^{H}_l(r)\,\rho^{TF}_{\bar{v},R-s}(r')}{\max\{r,r'\}}\,dr\,dr' + O(\bar{v}^2). \quad (24)$$

Next note

$$D(\tilde{\rho}-\rho^{TF}_{\bar{v},R-s},\tilde{\rho}-\rho^{TF}_{\bar{v},R-s}) \leqq (\tilde{\rho}-\chi_{[R+s,\infty)}\rho^{H},\tilde{\rho}-\chi_{[R+s,\infty)}\rho^{H}) + D(\chi_{[R+s,\infty)}\rho^{H}-\rho^{TF}_{\bar{v},R-s},\chi_{[R+s,\infty)}\rho^{H}-\rho^{TF}_{\bar{v},R-s})$$

and

$$D(\chi_{[R+s,\infty)}\rho^{H}-\rho^{TF}_{\bar{v},R-s},\chi_{[R+s,\infty)}\rho^{H}-\rho^{TF}_{\bar{v},R-s}) = \frac{1}{2}\int_{R-s}^{R+s}\int_{R-s}^{r+s}\frac{\rho^{TF}_{\bar{v},R-s}(r)\,\rho^{TF}_{\bar{v},R-s}(r')}{\max\{r,r'\}}\,dr\,dr'$$
$$+\int_{R-s}^{R+s}\rho^{TF}_{\bar{v},R-s}(r)\,dr\int_{R+s}^{\infty}\frac{1}{r'}(\rho^{H}(r')-\rho^{TF}_{\bar{v},R-s}(r'))\,dr'$$
$$+\frac{1}{2}\int_{R+s}^{0}\int_{R+s}^{\infty}\frac{(\rho^{H}(r)-\rho^{TF}_{\bar{v},R-s}(r))(\rho^{H}(r')-\rho^{TF}_{\bar{v},R-s}(r'))}{\max\{r,r'\}}\,dr\,dr'$$

$$\leqq \text{Const.}\left(\frac{1}{r^3}\Big|_{R+s}^{R-s}\frac{1}{r^4}\Big|_{R+s}^{R-s}+\frac{1}{r^3}\Big|_{R+s}^{R-s}\frac{1}{R^{5/2}}+\frac{1}{R^4}\right)=O\left(\frac{1}{R^{17/3}}\right)$$

where we used $\rho^H(r)\leqq\rho^{TF}_{\bar{\nu}, R-s}(r)+cr^{1/2}\varphi^{TF}_{\bar{\nu}, R-s}(r)^{3/4}$ ([9], (4.6)) and $s=R^{5/3}\leqq\frac{1}{4}R$ for $R\leqq\frac{1}{8}$, which is in agreement with our choice in the proof of Lemma 5.

We choose the same s in the following calculation.

$$\begin{aligned}
&D(\tilde{\rho}-\chi_{[R+s,\infty)}\rho^H, \tilde{\rho}-\chi_{[R+s,\infty)}\rho^H)\\
&\quad\leqq\frac{1}{2}\int_{R+s}^{R+2s}\int_{R+s}^{R+2s}\frac{\rho^H(r)\rho^H(r')}{\max\{r, r'\}}dr\,dr'\\
&\quad+\sum_{l=0}^{\infty}\int_{R+s}^{R+2s}\int_{x_2(l)}^{\infty}\frac{\beta^2 e^{-2\gamma r}\rho^H(r')}{\max\{r, r'\}}dr\,dr'\\
&\quad+\frac{1}{2}\sum_{l, l'=0}^{\infty}\int_{x_2(l)}^{\infty}\int_{x_2(l)}^{\infty}\frac{\beta_l^2 e^{-2\gamma r}\beta_{l'}^2 e^{-2\gamma r'}}{\max\{r, r'\}}dr\,dr'\\
&\quad\leqq\text{Const.}\left(\frac{1}{r^3}\Big|_{R+2s}^{R+s}\frac{1}{r^4}\Big|_{R+2s}^{R+s}+\frac{1}{r^3}\Big|_{R+2s}^{R+s}\bar{\nu}+\bar{\nu}^{5/3}\right)\\
&\qquad\qquad=O\left(\frac{1}{R^{17/3}}+\frac{\bar{\nu}}{R^{7/3}}+\bar{\nu}^{5/3}\right).
\end{aligned}$$

Thus

$$D(\tilde{\rho}-\rho^{TF}_{\bar{\nu}, R-s}, \tilde{\rho}-\rho^{TF}_{\bar{\nu}, R-s})=O\left(\frac{1}{R^{17/3}}+\frac{\bar{\nu}}{R^{7/3}}+\bar{\nu}^{5/3}\right). \tag{25}$$

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