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A NEW PHASE SPACE LOCALIZATION TECHNIQUE WITH APPLICATION TO THE SUM OF NEGATIVE EIGENVALUES OF SCHRÖDINGER OPERATORS

BY HEINZ SIEDENTOP AND RUDI WEIKARD

1. Introduction

Let H be the hamiltonian of N electrons in the field of a nucleus of charge Z, *i.e.*,

$$\mathrm{H}=\sum_{i=1}^{\mathrm{N}}\left(-\Delta_i-\frac{\mathrm{Z}}{|\mathbf{r}_i|}\right)+\sum_{\substack{i,\, j=1\\ i<j}}^{\mathrm{N}}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|} \tag{1}$$

selfadjointly realized in $\bigwedge_{i=1}^{\mathrm{N}}(\mathrm{L}^2(\mathbb{R}^3)\otimes\mathbb{C}^q)$, q being the number of spin states of a single electron. It has been shown (upper bound: Siedentop and Weikard [10], Bach [1]; lower bound: Siedentop and Weikard [9], Bach [1] based on a work of Hughes [3], [4]) that for fixed or negative degree of ionization $\lambda=1-\mathrm{N}/\mathrm{Z}$ – an assumption that we make throughout the whole paper without further mentioning – the following holds:

THEOREM 1:

$$\mathrm{E_Q}(\mathrm{Z},\,\mathrm{N})=\mathrm{E_{TF}}(1,\,\mathrm{N}/\mathrm{Z})\,\mathrm{Z}^{7/3}+\frac{q}{8}\mathrm{Z}^2+O(\mathrm{Z}^{47/24})$$

where $\mathrm{E_Q}(\mathrm{Z},\,\mathrm{N})=\inf\sigma(\mathrm{H})$ *and* $\mathrm{E_{TF}}(\mathrm{Z},\,\mathrm{N})$ *is the corresponding Thomas-Fermi energy.*

The upper bound is obtained by a variational calculation using eigenfunctions of the operator

$$\mathrm{H}_l^0=-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}-\frac{\mathrm{Z}}{r} \tag{2}$$

for small l, *i.e.*, $l<\mathrm{L}=[\mathrm{Z}^{1/12}]$, the integer part of $\mathrm{Z}^{1/12}$, and Macke orbitals, *i.e.*,

$$\varphi_{l,\,n}(r)=\left(\frac{\rho_l(r)}{\mathrm{N}_l}\right)^{1/2}\exp\left(i\pi k_{l,\,n}\int_0^r\frac{\rho_l}{\mathrm{N}_l}\,dt\right) \tag{3}$$

for $l \geqq L$ where $N_l = \int \rho_l$ and the $k_{l,n}$ differ for fixed l by even integers from each other. ρ_l is some suitable nonnegative function which may be interpreted as radial electron density in the angular momentum channel l (Siedentop and Weikard [8]).

For the lower bound one observes that

$$E_Q(Z, N) \geqq \sum_{l=0}^{\infty} q(2l+1)\,\mathrm{tr}(\tilde{H}_l)_- + \frac{1}{3} E_{TF}(Z, N) - \mathrm{const}\, Z^{5/3} \tag{4}$$

(Lieb [5], Siedentop and Weikard [9], Bach [1]). Here

$$\tilde{H}_l = -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - (\phi(r) - \mu)_+ = -\frac{d^2}{dr^2} - \phi_l, \tag{5}$$

$\phi - \mu$ being the Thomas-Fermi potential of the atom, *i.e.*, the solution of

$$\left(\frac{6\pi^2}{q}\right)^{2/3} \rho^{2/3}(r) = (\phi(r) - \mu)_+$$

$$\phi(r) = \frac{Z}{r} - \rho * \frac{1}{|\cdot|}(r)$$

under the condition $\int \rho = \min\{Z, N\}$, and ( ) denotes the restriction of the operator under consideration onto its negative spectral subspace. Again one distinguishes large and small angular momenta. For small l one may drop $\rho_{TF} * 1/|.|$ in (5) to obtain a bound which can be evaluated explicitly. However, the channels for large l were treated by a cumbersome WKB analysis (Hughes [3], [4], Siedentop and Weikard [9]).

The purpose of the present paper is to give a simpler proof of the lower bound using Macke orbitals requiring almost only known properties from the upper bound. We remark that $\{\varphi_{l,n} \mid n \in \mathbb{Z}\}$ is an orthonormal basis on $L^2(\mathbb{R}^+)$, if ρ_l is positive almost everywhere. Moreover the Macke orbitals yield a phase space localization through their « densities » ρ_l and their « momenta » $\pi k_{l,n}$.

The strategy of our proof is somewhat reminiscent to those of Berezin [2] and Lieb [5] who got upper and lower bounds using coherent states. Our idea is as follows. We break the one-particle operators $\tilde{H}_l$ into a sum of operators $H_{l,n}$ operating on almost orthogonal two-dimensional subspaces each of which has at most one bound state. The sum of the corresponding eigenvalues turns out to be the energy in the angular momentum channel l up to tolerable errors. This is the content of Section 2. The proof of the Scott type lower bound is basically the collection of the various pieces and an optimization of the various error bounds which is done in Section 3. The appendix is a collection of useful estimates most of which are transcriptions from [10] and [1].

2. Phase space localization by Macke orbitals

Now we introduce the Macke orbitals $\varphi_{l,\,n}$ of (3) explicitly by defining the radial densities ρ_l. Let

$$L_Z(r)=r(\phi(r)-\mu)_+^{1/2} \tag{6}$$

and define $k\in\mathbb{R}^+$ by $\beta_k=\max\{L_Z(r)^2\,|\,r\in\mathbb{R}^+\}$ where $\beta_x=x(x+1)$ in our case. For $l\leqq[k]-1$ we set

$$\rho_l(r)=q(2l+1)\begin{cases}\alpha^2 r^{2l+2}, & \text{if } 0\leqq r\leqq x_1,\\ \dfrac{1}{\pi r}(L_Z(r)^2-\beta_l)^{1/2}, & \text{if } x_1\leqq r\leqq x_2,\\ \beta^2\exp(-2Z^{2/3}r), & \text{if } x_2\leqq r.\end{cases} \tag{7}$$

The l and Z dependent numbers α^2 and β^2 ensure continuity of ρ_l at $x_1=r_1+T(\beta_l^{1/2}/Z)$ and $x_2=r_2-SZ^{-2/3}$ where T and S are suitable positive constants and r_1 and r_2 are the boundary points of the support of $(L_Z(r)^2-\beta_l)_+$. Remark that $x_1<x_2$ for Z large enough by (27). Furthermore let $n_l=N_l/(q(2l+1))$ and $k_{l,\,n}=2n$.

Now let V_l be the potential generated by the Fermi-Hellmann equations and the given radial densities ρ_l, *i.e.*,

$$-V_l=\alpha_l\rho_l^2 \qquad \text{for} \quad l\leqq[k]-1 \tag{8}$$

where $\alpha_l=\pi^2/q^2(2l+1)^2$ and let

$$H_l=-\frac{d^2}{dr^2}+V_l \tag{9}$$

in $L^2(0,\infty)$ with Dirichlet boundary conditions. The next lemma shows that the quantum mechanical problem involving V_l does not lower the sum of the negative eigenvalues — up to our required accuracy — for high enough angular momenta. Moreover angular momentum channels near to k may be omitted completely.

LEMMA 1. — *Let* $L=[Z^\delta]$ *and* $L'=[k-Z^\varepsilon]$ *with* $0<\varepsilon<2/9, 1/9<\delta<1/3$. *Then*

$$\sum_{l=L}^{\infty} q(2l+1)\,\mathrm{tr}(\tilde{H}_l)_-\geqq\sum_{l=L}^{L'-1} q(2l+1)\,\mathrm{tr}(H_l)_- -\mathrm{Const.}\,Z^{\max\{4/3+3\varepsilon,\ 19/9-\delta\}}.$$

Proof. — 1. $L'\leqq l$:

$\tilde{H}_l$ has the same negative eigenvalues as

$$-\frac{d^2}{dr^2}+\begin{cases}-\phi_l(r), & \text{if } r>0,\\ 0, & \text{if } r\leqq 0,\end{cases}$$

in $L^2((-\infty,0)\cup(0,\infty))$ with Dirichlet boundary conditions. Thus, using the Lieb-Thirring inequality ([7], Theorem 1) and by dropping the Dirichlet condition at zero we obtain

$$-\operatorname{tr}(\tilde{H}_l)_- \leqq \text{Const.} \int (\phi_l)_+^{3/2} = \text{Const.} \int_{r_1}^{r_2} \left(\frac{L_Z(r)^2 - \beta_l}{r^2}\right)^{3/2} dr$$

$$\leqq \text{Const.}\, Z^{3/2} \int_{r_1}^{r_2} (L_Z(r) - \beta_l^{1/2})^{3/2} dr$$

where we used (24) and $L_Z(r) \leqq \beta_k^{1/2}$.

We cut the last integral into two pieces, namely r_1 to the $RZ^{-1/3}$, where L_Z has its maximum, and $RZ^{-1/3}$ to r_2. Since $k - L' = O(Z^\varepsilon)$ the point r_2 is to the left of the smallest point of inflexion of L_Z with a distance of order $Z^{-1/3}$. Thus L_Z'' is negative on (r_1, r_2) and may be estimated from above and below by $-$Const. Z. By expansion we have

$$L_Z'(r) = (r - RZ^{-1/3})\, L_Z''(r')$$

$$L_Z(r) = \beta_k^{1/2} + \frac{1}{2}(r - RZ^{-1/3})^2\, L_Z''(r'')$$

with suitable points $r', r'' \in (r_1, r_2)$. Thus we have

(10) $$\text{Const.}\, Z^{1/2} (\beta_k^{1/2} - L_Z(r))^{1/2} \leqq |L_Z'(r)| \leqq \text{Const.}\, Z^{1/2} (\beta_k^{1/2} - L_Z(r))^{1/2}$$

and therefore by a change of variables

$$-\operatorname{tr}(\tilde{H}_l)_- \leqq \text{Const.}\, Z \int_{\beta_l^{1/2}}^{\beta_k^{1/2}} \frac{(x - \beta_l^{1/2})^{3/2}}{(\beta_k^{1/2} - x)^{1/2}} dx \leqq \text{Const.}\, Z (\beta_k^{1/2} - \beta_l^{1/2})^2.$$

Since $\tilde{H}_l \geqq 0$ for $l \geqq k$ summation yields

$$\sum_{l=L'}^{\infty} q(2l+1) \operatorname{tr}(\tilde{H}_l)_- = O(Z^{4/3 + 3\varepsilon}).$$

2. $L \leqq l < L'$:

The difference of the infima of the spectra of

$$\sum_{i=1}^{n_l^Q} \left(-\frac{d^2}{dr_i^2} + V_l(r_i)\right)$$

and

$$H_{\phi_l} := \sum_{i=1}^{n_l^Q} \left(-\frac{d^2}{dr_i^2} - \phi_l(r_i)\right)$$

may be estimated from above by

$$e_l = \int (\phi_l + V_l)_+ \rho_{\psi_l}$$

where ρ_{ψ_l} is the ground state density (or the densities of a minimizing sequence) of H_{ϕ_l}. Thus

$$\sum_{l=L}^{L'-1} q(2l+1) \operatorname{tr}(\tilde{H}_l)_- \geqq \sum_{l-L}^{L'-1} q(2l+1) \operatorname{tr}(H_l)_- - \sum_{l=L}^{L'-1} q(2l+1)\, e_l.$$

By the Hölder and the Lieb-Thirring inequality we have

$$(11)\quad \sum_{l=L}^{L'-1} q(2l+1)e_l$$

$$\leqq \left(\sum_{l=0}^{\infty} q(2l+1)\int_0^{\infty}\rho_{\psi_l}^3\,dr\right)^{1/3}\left(\sum_{l=L}^{L'-1} q(2l+1)\int_{(r_1,\,x_1)\cup(x_2,\,r_2)}\phi_l^{3/2}\,dr\right)^{2/3}$$

$$\leqq \text{Const.}\left(\sum_{l=0}^{\infty} q(2l+1)\,T_{\psi_l}\right)^{1/3}\left(\sum_{l=L}^{L'-1} q(2l+1)\int_{(r_1,\,x_1)\cup(x_2,\,r_2)}\left(\frac{L_Z(r)^2-\beta_l}{r^2}\right)^{3/2}\right)^{2/3}$$

where T_{ψ_l} is the kinetic energy of ψ_l. The first factor of the right hand side can be estimated by the cubic root of the ground state kinetic energy of $\sum_{i=1}^{N^Q}(-\Delta_i-(\phi(r_i)-\mu)_+)$ where $N^Q=\sum_{l=0}^{\infty} q(2l+1)n_l^Q$ using the fact that we treat an (effective) one-particle operator. This total kinetic energy, however, can be bounded by a Lieb-Simon type argument by Const. $Z^{7/3}$ (Lieb and Simon [6], Theorem III.2). The first factor on the right hand side of (11) is therefore $O(Z^{7/9})$. The integrals over the two intervals of the second factor of the right hand side of (11) can be estimated by

$$\int_{r_1}^{x_1}\frac{(L_Z(r)^2-\beta_l)^{3/2}}{r^3}dr \leqq (L_Z(x_1)^2-\beta_l)^{3/2}\,\frac{x_1-r_1}{r_1^3}=O(Z^2\,l^{-7/2})$$

$$\int_{x_2}^{r_2}\frac{(L_Z(r)^2-\beta_l)^{3/2}}{r^3}dr \leqq (L_Z(x_2)^2-\beta_l)^{3/2}\,\frac{r_2-x_2}{x_2^3}=O(Z^{5/6})$$

using (24)-(26), (28) and (29). Thus the left hand side of (11) is of the order of $Z^{19/9-\delta}$. ■

Now we introduce some notations. For $l\leqq[k]-1$ let

$$A_l=\frac{1}{n_l^2}\int_0^{\infty}\alpha_l\,\rho_l^3\,dr$$

$$B_l=\int_0^{\infty}\sqrt{\rho_l}'^2+V_l\,\rho_l\,dr$$

and

$$C_l=\int_0^{\infty}\sqrt{\rho_l}'^2\,dr\int_0^{\infty}-V_l\,\rho_l\,dr-\left(\int_0^{\infty}\sqrt{\rho_l}\,\sqrt{\rho_l}'(-V_l)^{1/2}\,dr\right)^2.$$

Observe that A_l and C_l are positive.

Since the Macke orbitals constitute an orthonormal basis we have by Bessels equality and by partial integration in the weak sense

$$H_l = \sum_{n=-\infty}^{\infty} H_{l,n} \tag{12}$$

where

$$H_{l,n} = |\varphi'_{l,n}\rangle\langle\varphi'_{l,n}| - |(-V_l)^{1/2}\varphi_{l,n}\rangle\langle(-V_l)^{1/2}\varphi_{l,n}|. \tag{13}$$

Remark that

$$\lambda_{l,n} = \frac{1}{2N_l}\{4n^2A_l + B_l - \sqrt{(4n^2A_l+B_l)^2+4C_l}\} \tag{14}$$

is the only negative eigenvalue of $H_{l,n}$.

LEMMA 2. — $\sum_{n=-\infty}^{\infty}\lambda_{l,n}$ *is absolutely convergent and*

$$\sum_{l=L}^{L'-1} q(2l+1)\sum_{n=-\infty}^{\infty}\lambda_{l,n}$$

$$\geqq -\frac{2}{3}\sum_{l=L}^{L'-1}\alpha_l^{-1/2}\int_0^\infty\left((\phi-\mu)_+ - \frac{l(l+1)}{r^2}\right)_+^{3/2} - \text{Const.}\, Z^{2-\delta/2}\log Z$$

for L, L′, *and* δ *as in Lemma* 1 *but with* $\varepsilon > 1/8$.

Proof. — We have for $L \leqq l < L'$ by inequalities (30) and (32)

$$0 \leqq \frac{\int \sqrt{\rho_l}'^2}{\int \alpha_l \rho_l^3} = O\left(\left(\frac{Z^2}{l^{3/2}} + Z^{17/12} l^{1/2}\right)\frac{1}{Z^{4/3}(k-l)^2}\right)$$

$$= \begin{cases} O(L^{-3/2}+Z^{-5/12}) \leqq 1/2, & \text{if } l \leqq k/2, \\ O(Z^{3/2-4/3-2\varepsilon}+Z^{1/4-2\varepsilon}) \leqq 1/2, & \text{if } l > k/2, \end{cases}$$

if $\varepsilon > 1/8$ and Z sufficiently large. Thus, by definition of V_l,

$$\frac{1}{2}n_l^2 \leqq \frac{-B_l}{A_l} = n_l^2\left(1 - \frac{\int\sqrt{\rho_l}'^2}{\int\alpha_l\rho_l^3}\right) \leqq n_l^2. \tag{15}$$

Now for n such that $\gamma_{l,n} := ||2n| - \sqrt{-B_l/A_l}| \geqq 4$ the estimate

$$q(2l+1)\lambda_{l,n} \geqq \frac{1}{2n_l}\left\{B_l + 4n^2A_l - |B_l + 4n^2A_l| - \frac{2C_l}{A_l}\frac{1}{|4n^2+B_l/A_l|}\right\} \tag{16}$$

is appropriate, otherwise we use

$$q(2l+1)\lambda_{l,\,n} \geqq \frac{1}{2n_l}\{B_l+4n^2 A_l - |B_l+4n^2 A_l| - 2\sqrt{C_l}\}. \tag{17}$$

By monotonicity of the function $1/|x^2-c^2|$ in the intervals $(0, |c|)$ and $(|c|, \infty)$ we estimate as follows

$$\frac{1}{n_l}\sum_{\substack{n=-\infty \\ \gamma_{l,\,n}\geqq 4}}^{\infty} \frac{C_l}{A_l}\frac{1}{|4n^2+B_l/A_l|} \leqq \text{Const.}\frac{C_l}{n_l^2 A_l}\log n_l = O\left(\left(\frac{Z^2}{l^{3/2}}+Z^{17/12}l^{1/2}\right)\log Z\right) \tag{18}$$

by (15), (30), and (34).

Moreover

$$\frac{1}{n_l}\sum_{\substack{n=-\infty \\ \gamma_{l,\,n}<4}}^{\infty} \sqrt{C_l} = O\left(\frac{Z^{5/3}}{l^{3/4}}+Z^{33/24}l^{1/4}\right), \tag{19}$$

since we have only finitely many summands and by (30), (32) and (34).

The main terms of (16) and (17) yield

$$-\frac{1}{n_l}\sum_{\substack{n=-\infty \\ 4n^2<-B_l/A_l}}^{\infty} (B_l+4n^2 A_l) = -\frac{1}{n_l}A_l\left(-4\nu_l^2+8\sum_{n=1}^{[\nu_l]}(n^2-\nu_l^2)\right) \tag{20}$$

with $\nu_l=\sqrt{-B_l/4A_l}$. Thus (20) becomes

$$\begin{aligned} \int \alpha_l \rho_l^3\left(\frac{16}{3}\left(\frac{\nu_l}{n_l}\right)^3 + O\left(\frac{\nu_l}{n_l^3}\right)\right) &\leqq \frac{2}{3}\int \alpha_l \rho_l^3 (1+O(n_l^{-2})) \\ &\leqq \frac{2}{3}\int \alpha_l^{-1/2}(\phi_l)_+^{3/2} + \frac{2}{3}\int_0^{x_1} \alpha_l \rho_l^3 + \frac{2}{3}\int_{x_2}^{\infty} \alpha_l \rho_l^3 + \text{Const.}\, n_l^{-2}\int \alpha_l \rho_l^3 \\ &\leqq \frac{2}{3}\int \alpha_l^{-1/2}(\phi_l)_+^{3/2} + \text{Const.}\,(Z^2 l^{-5/2} + n_l^{-2}\int \alpha_l \rho_l^3) \end{aligned} \tag{21}$$

using (15), (22), (23) and the Fermi-Hellmann equation. Thus, collecting terms, we obtain from (16), (17), (18), (19), and (21)

$$\sum_{n=-\infty}^{\infty} q(2l+1)\lambda_{l,\,n} \geqq -\frac{2}{3}\int \alpha_l^{-1/2}(\phi_l)_+^{3/2} - \text{Const.}\left(\frac{Z^2\log Z}{l^{3/2}} + Z^{17/12}l^{1/2}\log Z + n_l^{-2}\int \alpha_l \rho_l^3\right).$$

Summation over l using (31) yields the desired result. ■

The following theorem is a basic fact of our microlocalization.

THEOREM 2. — *Let* H_l *be given as in* (9) *and* $\lambda_{l,n}$ *as in* (14). *Then*

$$\operatorname{tr}(H_l)_- \geqq \sum_{n=-\infty}^{\infty} \lambda_{l,n}.$$

Proof. — Let M be the set of all trace class operators d with finite kinetic energy and $0 \leqq d \leqq 1$. Then

$$\operatorname{tr}(H_l)_- = \inf\{\operatorname{tr}(H_l d) \mid d \in M\} \geqq \sum_{n=-\infty}^{\infty} \inf\{\operatorname{tr}(H_{l,n} d) \mid d \in M\} = \sum_{n=-\infty}^{\infty} \operatorname{tr}(H_{l,n})_-$$

where $H_{l,n}$ is given by (13). The claim follows now from the fact that $\lambda_{l,n}$ is the only negative eigenvalue of $H_{l,n}$. ■

3. Application to the Scott problem

By the above arguments we are now in a position to bound the hamiltonian (1) from below.

THEOREM 3:

$$H \geqq E_{TF}(1, N/Z) Z^{7/3} + \frac{q}{8} Z^2 - \text{Const.}\, Z^{53/27}.$$

Proof. — Estimating the eigenvalues of $\tilde{H}_l$ for small l, *i.e.*, $l < L$, by the eigenvalues of H_l^0 we obtain

$$\sum_{l=0}^{L-1} q(2l+1)\operatorname{tr}(\tilde{H}_l)_- \geqq -\frac{qZ^2}{2} L + \frac{q}{8} Z^2 - \text{Const.}\, Z^2 L^{-1}$$

$$\geqq -\frac{2}{3} \sum_{l=0}^{L-1} \int \alpha_l^{-1/2} \left((\phi-\mu)_+ - \frac{(l+(1/2)^2}{r^2} \right)_+^{3/2} + \frac{q}{8} Z^2 - \text{Const.}\, (Z^{2-\delta} + Z^{5/3+2\delta})$$

using page 190, second but last inequality, of [9] and replacing Z/r by $(\phi-\mu)_+$ analogously to the proof of Lemma 12, second part, of [9]. By Lemmata 1 and 2 and Theorem 2 we have for $\varepsilon = 1/6$.

$$\sum_{l=L}^{\infty} q(2l+1)\operatorname{tr}(\tilde{H}_l)_- \geqq -\frac{2}{3} \sum_{l=L}^{\infty} \int \alpha_l^{-1/2} \left((\phi-\mu)_+ - \frac{(l+(1/2))^2}{r^2} \right)_+^{3/2}$$
$$- \text{Const.}\, (Z^{19/9-\delta} + (Z^{2-\delta/2} + Z^{23/12}) \log Z)$$

where we used again an argument analogously to Lemma 12, first part, of [9] to substitute $l(l+1)$ by $(l+(1/2))^2$.

Optimizing δ yields $\delta = 4/27$ and the error terms of order $Z^{53/27}$. Then Poisson summation — generating errors of order $Z^{5/3}$ only (*see* [10]) — and formula (4) yield the desired result. ■

A. Some useful formulae

Throughout this appendix assume $L \leqq l \leqq [k] - 1$ and $Z \gg 1$.

By explicit integration

$$\alpha_l \int_0^{x_1} \rho_l^3 = O\left(\frac{Z^2}{l^{5/2}}\right), \tag{22}$$

$$\alpha_l \int_{x_2}^{\infty} \rho_l^3 = O(Z^{7/6}\, l). \tag{23}$$

The following results are easily transcribed from [10], Lemma C.1, formulae (3.9), (3.12), and (3.13), and [1], Lemma 18, 19, and 20.

$$\frac{\beta_l}{Z} \leqq r_1 \leqq \text{Const.}\, \frac{\beta_l}{Z}, \tag{24}$$

$$\frac{\text{Const.}}{l} \leqq r_2 \leqq \frac{\text{Const.}}{l} \qquad \text{for} \quad \lambda \leqq 0, \tag{25}$$

$$\frac{\text{Const.}}{Z^{1/3}} \leqq r_2 \leqq \frac{\text{Const.}}{Z^{1/3}} \qquad \text{for} \quad \lambda > 0. \tag{26}$$

Furthermore

$$x_1 \leqq R Z^{-1/3} - \text{Const.}\, Z^{-1/2} < R Z^{-1/3} + \text{Const.}\, Z^{-1/2} \leqq x_2, \tag{27}$$

$$L_Z(x_1)^2 - \beta_l \leqq T\, \beta_l^{1/2}, \tag{28}$$

$$L_Z(x_2)^2 - \beta_l \leqq \text{Const.}\, Z^{1/3}, \tag{29}$$

$$\int \sqrt{\rho_l}'^2 = O\left(\frac{Z^2}{l^{3/2}} + Z^{17/12}\, l^{1/2}\right), \tag{30}$$

$$\sum_{l=L}^{[k]-1} \frac{\alpha_l \int \rho_l^3}{n_l^2} \leqq \text{Const.} \sum_{l=L}^{[k]-1} \frac{Z^{4/3}(k-l)^2}{(k-l)^2} = O(Z^{5/3}). \tag{31}$$

Next we note

$$\text{Const.}\, Z^{4/3}(k-l)_+^2 \leqq \int \alpha_l\, \rho_l^3 \leqq \text{Const.}\, Z^{4/3}(k-l)_+^2. \tag{32}$$

Proof. — The upper bound is a transcription as above. The lower bound requires a separate treatment: Note the scaling $L_{\lambda,Z}(r) = Z^{1/3} L_{\lambda,1}(Z^{1/3} r)$. Denote the unique maximum of $L_{\lambda,1}$ (*see* [10], Lemma A.1, and [1], Lemma 5) by R. (At this point we make explicit the λ dependence of L_Z.) This yields that there are positive constants c_1, c_2 such that $L_{\lambda, Z}(r)^2 \geqq c_1 Z r$ for $r \leqq c_2 Z^{-1/3}$. Moreover by [1], Lemma 3.(ii) and [10], formula (B.4)

$$L'_{\lambda, Z}(r) < L'_{0, Z}(r) \leqq \text{Const.} \left(\frac{Z}{r}\right)^{1/2} \qquad \text{for} \quad r \leqq c_2 Z^{-1/3}$$

possibly by decreasing c_2.

For $\beta_l \leqq c_3^2 \beta_k$ with c_3 positive but sufficiently small

$$\int \alpha_l \rho_l^3 \geqq \text{Const.}\, l \int_{x_1}^{c_2 Z^{-1/3}} \frac{\sqrt{L_Z(r)^2 - \beta_l}^{\,3}}{r^3 L'_Z(r)} L'_Z(r)\, dr. \tag{33}$$

which may be estimated from below by

$$\text{Const.}\, l \int_{L_Z(x_1)}^{L_Z(c_2 Z^{-1/3})} Z^2 \frac{(y^2 - \beta_l)^{3/2}}{y^5} dy \geqq \text{Const.}\, Z^2 \int_a^b \frac{(x^2-1)^{3/2}}{x^5} dx \geqq Z^{4/3} (k-l)^2,$$

since by (28) for suitable c_3

$$a := \frac{L_Z(x_1)}{\beta_l^{1/2}} \leqq 1 + T < \frac{\text{Const.}}{c_3} \leqq \frac{L_Z(c_2 Z^{-1/3})}{c_3 \beta_k^{1/2}} \leqq \frac{L_Z(c_2 Z^{-1/3})}{\beta_l^{1/2}} =: b.$$

For $\beta_l > c_3^2 \beta_k$ the integral $\int \alpha_l \rho_l^3$ – noting $x_1 \geqq \text{Const.}\ Z^{-1/3}$ – may be estimated from below by

$$\text{Const.}\, l Z^{1/2} \int_{L_Z(x_1)}^{L_Z(R Z^{-1/3})} \frac{(L^2 - \beta_l)^{3/2}}{(\beta_k^{1/2} - L)^{1/2}} dL$$

because of (10). Moreover, since

$$c := \left(\frac{\beta_k^{1/2} - L_Z(x_1)}{\beta_k - \beta_l}\right)^{1/2} \geqq (1 - T/2)^{1/2},$$

we obtain

$$\int \alpha_l \rho_l^3 \geqq \text{Const.}\, l^{5/2} Z^{1/2} (k-l)^2 \int_0^c (1-x^2)^{3/2} dx \geqq \text{Const.}\, Z^{4/3} (k-l)^2,$$

which proves (32).

Finally

$$\text{Const.}\,(k-l) \leqq n_l \leqq \text{Const.}\,(k-l). \tag{34}$$

Proof. – In this case the lower bound is a transcription as above, and the upper bound requires a separate treatment: By direct integration

$$\int_0^{x_1} \rho_l + \int_{x_2}^{\infty} \rho_l = q(2l+1)\, O(1).$$

Now we estimate the middle term: First let $l \leqq k/2$. We split the integral at $RZ^{-1/3}$ and the use for $\phi(r)$ the upper bound Z/r on the left part and Const.$/r^4$ (Sommerfeld solution) on the right part. By dropping the β_l one directly obtains the desired inequality. For $k/2 \leqq l$ we split the interval of integration at $RZ^{-1/3}$ once more, but by using (10) we obtain

$$\int_{x_1}^{x_2} \rho_l \leqq \text{Const.} \frac{Z^{1/3} k^{1/2}}{Z^{1/2}} \int_{\sqrt{\beta_l}}^{\sqrt{\beta_k}} \left(\frac{L - \sqrt{\beta_l}}{\sqrt{\beta_k} - L} \right)^{1/2} dL \leqq \text{Const.}\,(k-l).$$

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