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Improved constraints on states bound by a class of potentials

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Abstract. Recent work on states bound by a central potential whose Laplacian is positive is extended to cover a wider class of potentials for which energy level ordering theorems can be proved. This class includes *power law potentials* in particular. Constraints on the moments of the radial distance are improved and similarly for the kinetic energy. These constraints are shown to provide tight bounds on the energies of ground states for power law potentials, and on their variation with angular momentum. They are also used to bound the position of the maximum of the wavefunction for these states.

1. Introduction

In a recent work one of us (Common 1985) studied properties of states bound by a central potential whose Laplacian is positive. Although this was motivated by heavy quark spectroscopy, since both ψ and γ systems are well described by a non-relativistic treatment, it has applications in other areas of physics as discussed by Baumgartner *et al* (1984).

The above study used a result which is crucial to the proof of energy level ordering theorems (Baumgartner *et al* 1984). This is that for a central potential $V(r)$ whose Laplacian $r^{-2}(\mathrm{d}/\mathrm{d}r)(r^2\,\mathrm{d}V/\mathrm{d}r)>0$ for all $r>0$,

$$-\left(\frac{u'_{0,l}(r)}{u_{0,l}(r)}\right)' > \frac{l+1}{r^2} \qquad r>0 \tag{1.1}$$

where $u_{0,l}(r)$ is the reduced wavefunction for the ground state of angular momentum l. The converse of (1.1) holds for potentials for which there exists an r_0 such that $r^{-2}(\mathrm{d}/\mathrm{d}r)(r^2\,\mathrm{d}V/\mathrm{d}r)<0$ for $r<r_0$ and $\mathrm{d}V/\mathrm{d}r<0$ for $r\geqslant r_0$. The level ordering result is that, if $E(n,l)$ is the energy of the level with angular momentum l and n is the number of nodes of the wavefunction, then

$$E(n,l) \gtrless E(n-1,l+1) \tag{1.2}$$

with the upper (lower) inequality corresponding to the case of positive (negative) Laplacian.

These results have been generalised recently by Baumgartner *et al* (1985) to other classes of potential by transforming to the variable $z=r^\alpha$. For example, for a positive potential such that

$$D_\alpha V(r) \equiv \frac{\mathrm{d}^2V}{\mathrm{d}r^2} + (5-3\alpha)\frac{1}{r}\frac{\mathrm{d}V}{\mathrm{d}r} + 2(1-\alpha)(2-\alpha)\frac{V(r)}{r^2} > 0 \tag{1.3}$$

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for all $r>0$ and some $2>\alpha>1$, then

$$E(n, l)>E(n-1, l+\alpha). \tag{1.4}$$

The condition (1.3) is chosen so that the Laplacian of the 'potential' of the Schrödinger equation in the 'transformed' variable z has positive Laplacian. The ground-state wavefunction in the transformed variable then satisfies a condition corresponding to (1.1) and inequality (1.4) follows.

It is the purpose of this work to extend the results of Common (1985) to classes of potentials considered by Baumgartner *et al* (1985). In § 2, we describe in more detail the transformation from the energy eigenvalue equation for $V(r)$ to the corresponding equation in the z variable. We then derive a relation between the moments of r and the moments of z in the transformed system and similarly for the corresponding kinetic energies. In § 3, we generalise the moment inequalities given previously and also the corresponding inequalities on the kinetic energy. We apply these results in § 4 to obtain tight bounds on the variation of energy with angular momentum for power law potentials, while in the final section we derive improved bounds on the position of the unique maximum of the ground-state wavefunction $u_{0,l}(r)$ and also draw some conclusions.

2. The transformed system

The reduced wave $u_{n,l}(r)$ corresponding to energy $E(n, l)$ satisfies the equation

$$-\frac{d^2}{dr^2}u_{n,l}(r)+\left(\frac{l(l+1)}{r^2}+V(r)\right)u_{n,l}(r)=E(n, l)u_{n,l}(r). \tag{2.1}$$

When written in terms of the transformed variable $z=r^\alpha$, it becomes (Baumgartner *et al* 1985)

$$-\frac{d^2}{dz^2}w_{n,\lambda}(z)+\left(\frac{\lambda(\lambda+1)}{z^2}+U(z)\right)w_{n,\lambda}(z)=0 \tag{2.2}$$

where

$$U(z)\equiv(V(r)-E(n, l))/(\alpha^2z^{2-2/\alpha}) \tag{2.3a}$$

$$\lambda\equiv(2l-\alpha+1)/2\alpha \qquad w_{n,\lambda}(z)\equiv(\alpha r^{\alpha-1})^{1/2}u_{n,l}(r). \tag{2.3b}$$

The 'moments' of the original and transformed systems are then related in the following manner:

$$\int_0^\infty w_{n,\lambda}^2(z)z^k\,dz=\alpha^2\int_0^\infty r^{2\alpha-2+k\alpha}u_{n,l}^2(r)\,dr \qquad k=0, 1, 2, \ldots. \tag{2.4}$$

Similarly from (2.3a)

$$\begin{aligned}\frac{1}{2}\int_0^\infty z\frac{dU(z)}{dz}w_{n,\lambda}^2(z)\,dz &=\frac{1}{2\alpha}\int_0^\infty(2-2\alpha)(V(r)-E(n, l))u_{n,l}^2(r)\,dr+\frac{1}{2\alpha}\int_0^\infty r\frac{dV}{dr}u_{n,l}^2(r)\,dr\\ &=-\frac{(1-\alpha)}{\alpha}T_{n,l}+\frac{1}{\alpha}T_{n,l}=T_{n,l}\end{aligned} \tag{2.5}$$

where we have used the virial theorem for $T_{n,l}$, the kinetic energy of the state of energy $E(n,l)$ and taken $u_{n,l}(r)$ to be normalised to unity. The kinetic energy $\mathbb{T}_{n,\lambda}$ of the 'transformed' system is also given by the virial theorem to be

$$\mathbb{T}_{n,\lambda}=\frac{1}{2}\int_0^\infty z\frac{\mathrm{d}U(z)}{\mathrm{d}z}w_{n,\lambda}^2(z)\,\mathrm{d}z\left(\int_0^\infty w_{n,\lambda}^2(z)\,\mathrm{d}z\right)^{-1} \tag{2.6}$$

where it should be noted from (2.4) with $k=0$ that, in general, $w_{n,\lambda}(z)$ will *not* be normalised to unity. Combining (2.5) with (2.6),

$$\mathbb{T}_{n,\lambda}=T_{n,l}\left(\alpha^2\int_0^\infty r^{2\alpha-2}u_{n,l}^2(r)\,\mathrm{d}r\right)^{-1}. \tag{2.7}$$

3. Inequalities

Baumgartner *et al* (1985) defined classes of potentials $V(r)$ for which the Laplacian of $U(z)$ had a definite sign and hence a condition on $w_{0,l}(z)$ corresponding to (1.1) held. We form these classes into two sets as follows.

Set A. For all $r>0$ one of the following conditions holds:
(i) $D_\alpha V(r)>0,\ 1<\alpha<2,\ V(r)>0$,
(ii) $D_\alpha V(r)>0,\ \alpha<1,\ V(r)<0$,
(iii) $[r^2\,\mathrm{d}^2/\mathrm{d}r^2+(3-2\alpha)\,\mathrm{d}/\mathrm{d}r]V(r)>0,\ 1<\alpha<2, \mathrm{d}V/\mathrm{d}r>0$,
where $D_\alpha V(r)$ is defined in (1.3).

Notice that, in case (iii), if V belongs to A for $\alpha=\alpha_0$ it also belongs to A for any $\alpha<\alpha_0$.

Set B. For all $r>0$ one of the following conditions holds:
(i) $D_\alpha V(r)<0, \alpha>2$ or $<1,\ V(r)>0$,
(ii) $D_\alpha V(r)<0, 1<\alpha<2,\ V(r)<0$,
(iii) $[r^2\,\mathrm{d}^2/\mathrm{d}r^2+(3-2\alpha)\,\mathrm{d}/\mathrm{d}r]V(r)<0, \alpha>2$.

Note that a given potential can belong to both set A and set B for different choices of α. For instance, in the special case of power law potentials $V_\nu(r)=\varepsilon(\nu)r^\nu$:
(a) $\nu>2$, V_ν belongs to A with $\alpha=2$ and to B with $\alpha=\frac{1}{2}(\nu+2)$,
(b) $2>\nu>0$, V_ν belongs to B with $\alpha=2$ and to A with $\alpha=\frac{1}{2}(\nu+2)$,
(c) $0>\nu>-1$, V_ν belongs to A with $\alpha=1$ and to B with $\alpha=\nu+2$,
(d) $-1>\nu$, V_ν belongs to A with $\alpha=\nu+2$ and to B with $\alpha=1$.

It was shown by Baumgartner *et al* (1985) that

$$-\left(\frac{w_{0,\lambda}'(z)}{w_{0,\lambda}(z)}\right)'\gtrless\frac{(\lambda+1)}{z^2} \tag{3.1}$$

where the upper (lower) inequality holds for potentials in set A(B). Using the methods of Common (1985), the inequalities (3.1) may be used to prove the following moment inequalities for all $\lambda>0$. If $V(r)$ belongs to set A,

$$(2\lambda+2+k)\{z^{k-1}\}_\lambda\{z^n\}_\lambda\leqslant(2\lambda+2+n)\{z^k\}_\lambda\{z^{n-1}\}_\lambda \tag{3.2}$$

where $\{z^t\}_\lambda\equiv\int_0^\infty z^t w_{0,\lambda}^2(z)\,\mathrm{d}z$ and $n>k$ are any pair of real numbers such that all the integrals concerned exist. When $V(r)$ belongs to set B the inequality is reversed.

Transforming these results back to the original variable we obtain the following theorem.

Theorem. If $V(r)$ belongs to set $\binom{\mathrm{A}}{\mathrm{B}}$ then for all $l \geqslant 0$, $n > k$ for which the integrals concerned exist,

$$(2l+1+\alpha+k\alpha)\langle r^{2(\alpha-1)+n\alpha}\rangle_{0,l}\langle r^{2(\alpha-1)+(k-1)\alpha}\rangle_{0,l} \lesseqgtr (2l+1+\alpha+n\alpha)\langle r^{2(\alpha-1)+k\alpha}\rangle_{0,l}\langle r^{2(\alpha-1)+(n-1)\alpha}\rangle_{0,l} \tag{3.3}$$

where

$$\langle r^k\rangle_{0,l} \equiv \int_0^\infty u_{0,l}^2(r) r^k \, \mathrm{d}r.$$

For case A these bounds complement the usual 'moment' inequalities,

$$\langle r^{2(\alpha-1)+n\alpha}\rangle_{0,l}\langle r^{2(\alpha-1)+(k-1)\alpha}\rangle_{0,l} \geqslant \langle r^{2(\alpha-1)+k\alpha}\rangle_{0,l}\langle r^{2(\alpha-1)+(n-1)\alpha}\rangle_{0,l}. \tag{3.4}$$

It can also be checked that those corresponding to $\alpha > 1$ are more constraining than those for $\alpha = 1$. For case B the inequalities (3.3) improve on (3.4). These inequalities will be used in § 5.

We now consider the kinetic energies. Using again the methods of Common (1985) the inequality (3.1) may be used to prove that if $V(r)$ is in set $\binom{\mathrm{A}}{\mathrm{B}}$ then

$$\mathbb{T}_{0,\lambda} \gtrless (\lambda+1)(\lambda+\tfrac{1}{2})\{z^{-2}\}_{0,\lambda}/\{1\}_{0,\lambda}. \tag{3.5}$$

The proof is based on the following integration by parts:

$$\int_0^\infty (w'(z))^2 \, \mathrm{d}z = \int_0^\infty \left(\frac{w'(z)}{w(z)}\right) w(z) w'(z) \, \mathrm{d}z = -\frac{1}{2}\int_0^\infty \left(\frac{w'(z)}{w(z)}\right)' w^2(z) \, \mathrm{d}z$$

followed by the use of inequality (1.1). Transforming back to the original variables and using (2.4) with $k = -2$ we obtain the following.

Theorem. If $V(r)$ belongs to set $\binom{\mathrm{A}}{\mathrm{B}}$, then

$$T_{0,l} \gtrless \left(l + \frac{\alpha+1}{2}\right)(l+\tfrac{1}{2})\langle r^{-2}\rangle_{0,l}. \tag{3.6}$$

It is important to remember that the moment inequalities (3.3) and the bounds (4.2) on the kinetic energy have been proved for the *ground* states of given angular momentum. However, the lower bounds in the latter case can be extended to excited states as shown by the following result.

Corollary. For potentials belonging to set A, the lower bounds (3.6) can be extended to excited states, i.e.

$$T_{n,l} > \left(l + \frac{\alpha+1}{2}\right)(l+1)\langle r^{-2}\rangle_{n,l} \qquad n,l = 0, 1, 2, \ldots. \tag{3.6a}$$

The proof of this corollary is given in appendix 1.

4. Energy bounds

For power law potentials $V(r) = \varepsilon(\nu) r^\nu$, we can use (3.6) to derive the following set of bounds:

(a) $\nu > 2$

$$(l+\tfrac{1}{2})(l+\tfrac{3}{2})\langle r^{-2}\rangle_{0,l} < T_{0,l} < (l+\tfrac{1}{2})[l+\tfrac{1}{4}(\nu+4)]\langle r^{-2}\rangle_{0,l} \tag{4.1a}$$

(b) $0<\nu<2$

$$(l+\tfrac{1}{2})\left(l+\frac{\nu+4}{4}\right)\langle r^{-2}\rangle_{0,l}<T_{0,l}<(l+\tfrac{1}{2})(l+\tfrac{3}{2})\langle r^{-2}\rangle_{0,l} \qquad (4.1b)$$

(c) $-1<\nu<0$

$$(l+\tfrac{1}{2})(l+1)\langle r^{-2}\rangle_{0,l}<T_{0,l}<(l+\tfrac{1}{2})\left(l+\frac{\nu+3}{2}\right)\langle r^{-2}\rangle_{0,l} \qquad (4.1c)$$

(d) $-2<\nu<-1$

$$(l+\tfrac{1}{2})\left(l+\frac{\nu+3}{2}\right)\langle r^{-2}\rangle_{0,l}<T_{0,l}<(l+\tfrac{1}{2})(l+1)\langle r^{-2}\rangle_{0,l}. \qquad (4.1d)$$

These are obtained by choosing, for a given ν, values of $\alpha=\alpha_1$ or α_2 so that $V(r)$ belongs to set A or B, respectively, and which give optimal bounds. For example, when $\nu>2$, one takes $\alpha_1=2$ and $\alpha_2=(\nu+2)/2$ as stated earlier.

The inequalities (4.1) give tight bounds on the variation of $E(0,l)$ with l since from the virial theorem, for the above power law potentials,

$$E(n,l)=\left(\frac{2+\nu}{\nu}\right)T_{n,l} \qquad (4.2)$$

and from the Feynman–Hellmann theorem (Feynman 1979, Hellmann 1937)

$$\partial E(n,l)/\partial l=(2l+1)\langle r^{-2}\rangle_{n,l}. \qquad (4.3)$$

For example, from (4.1b) we find for $0<\nu<2$ that

$$[l+(\nu+4)/4]\partial E(0,l)/\partial l\leqslant[2\nu/(2+\nu)]E(0,l)\leqslant(l+\tfrac{3}{2})\partial E(0,l)/\partial l. \qquad (4.4)$$

Integrating

$$[(L+\tfrac{3}{2})/(l+\tfrac{3}{2})]^{2\nu/(\nu+2)}\leqslant E(0,L)/E(0,l)$$
$$\leqslant\{[L+(\nu+4)/4]/[l+(\nu+4)/4]\}^{2\nu/(\nu+2)} \qquad L>l. \qquad (4.5)$$

To show that these are significant bounds, we consider the linear potential $V(r)=r$ for which the lowest energy levels have been evaluated numerically (Antippa *et al* 1978). These numerical values have been used to calculate $E(0,L)/E(0,l)$ for $l=0$ and $L=1$ to 6 and compared in table 1 with the bounds given by (4.5). It will be seen that for angular momentum as high as $L=6$, the bounds (4.5) allow us to determine $E(0,L)$ from $E(0,0)$ to within an error of 5%.

Table 1. The bounds to $E(0,L)/E(0,l)$ for $l=0$ compared with computed values.

L	Lower bound	Numerical value	Upper bound
1	1.406	1.438	1.480
2	1.759	1.817	1.891
3	2.080	2.160	2.261
4	2.378	2.478	2.603
5	2.658	2.777	2.924
6	2.924	3.060	3.228

One can also use (4.5) to obtain absolute bounds by letting L tend to infinity and using the fact that

$$\lim_{L\to\infty} E(0, L)/(L^{2\nu/(\nu+2)}) = (|\nu|/2)^{2/(\nu+2)}(\nu+2)/\nu. \tag{4.6}$$

In this way one obtains

(a) $0 \leqslant \nu \leqslant 2$:

$$E(0, l) \leqslant [(\nu+2)/\nu](\nu/2)^{2/(\nu+2)}(l+\tfrac{3}{2})^{2\nu/(\nu+2)} \tag{4.7}$$

$$E(0, l) \geqslant [(\nu+2)/\nu](\nu/2)^{2/(\nu+2)}[l+(\nu+4)/4]^{2\nu/(\nu+2)}. \tag{4.8}$$

(b) $2 \leqslant \nu < \infty$:

$$E(0, l) \leqslant [(\nu+2)/\nu](\nu/2)^{2/(\nu+2)}[l+(\nu+4)/4]^{2\nu/(\nu+2)} \tag{4.9}$$

$$E(0, l) \geqslant [(\nu+2)/\nu](\nu/2)^{2/(\nu+2)}(l+\tfrac{3}{2})^{2\nu/(\nu+2)}. \tag{4.10}$$

The most unfavourable case of these bounds are when $l=0$ and we then obtain

(i) for a linear potential ($\nu = 1$),

$$2.193\,01 \leqslant E(0, 0) \simeq 2.338\,11 \leqslant 2.4764$$

(ii) for a quartic potential ($\nu = 4$),

$$3.24 \leqslant E(0, 0) \simeq 3.8 \leqslant 4.77.$$

More refined upper bounds can be obtained, however, using a variational approach by taking $u = r^m \exp(-\lambda r^2)$ as a trial function with m, λ variational parameters. One gets, for $\nu > 2$,

$$E(0, l) \leqslant [(\nu+2)/\nu](\nu/2)^{2/(\nu+2)}[l+\tfrac{1}{2}+\tfrac{1}{2}(\nu+2)^{1/2}]^{2\nu/\nu+2}. \tag{4.11}$$

For the quartic potential this gives

$$E(0, 0) \leqslant 3.91$$

which is to be compared with the previous bound above.

For the case $0 < \nu < 2$, (4.11) has to be replaced by a more complicated expression. However, for $\nu = 1$, a bound which is significant for l small is obtained by multiplying (4.11) by $(\pi/3)^{1/2}$ and then

$$E(0, 0) \leqslant 2.38.$$

These results can be used to prove 'concavity' properties such as

$$2E(0, l) > E(0, l+1) + E(0, l-1)$$

for potentials $V = r^\alpha$, $0 \leqslant \alpha \leqslant 2$.

5. The maximum of the wavefunction and conclusions

In this section we use the moment inequalities (3.3) to improve the bounds on the position of the peak of the reduced ground-state wavefunctions obtained previously. The reduced ground-state wavefunction $u_{0,l}(r)$ is non-zero for $r > 0$ and (if assumed positive) has a single maximum at $r = r_{Ml}$, say. Previously we obtained upper and lower bounds to r_{Ml} which are proportional to $\langle r \rangle_{0,l}$. They were not particularly precise but the ratio of the upper and lower bounds tended to $\sqrt{3}$ as $l \to \infty$, so for large l they were quite reasonable.

An improvement on these results is given by the following theorem.

Theorem. If $V(r)$ belongs to set A defined in § 3 for a given $\alpha > 1$, then

$$\langle r\rangle_{0,l}\left(\frac{[(2l+2)^{1/2}+\sqrt{\alpha}]^2}{2l-\alpha+3}\right)^{1/\alpha} \geq r_{Ml} \geq \langle r\rangle_{0,l}\left(\frac{[(2l+2)^{1/2}-\sqrt{\alpha}]^2}{2l+3}\right)^{1/\alpha} \tag{5.1}$$

when $l > (3-\alpha)/2$ in the case of the left-hand inequality and when $l > (\alpha-2)/2$ for the right-hand inequality.

The proof is given in appendix 2 and (5.1) has the nice property that, as $l \to \infty$, the ratio of the upper and lower bounds tends to unity so that in this limit $r_{Ml} \to \langle r\rangle_{0,l}$. The bounds also become tighter as α is increased from unity (in fact, an optimum value for α can be found), and they are in accord with the fact (Common 1985) that the relative width of the peak of $u_{0,l}(r)$ tends to zero as $l \to \infty$.

In this work we have generalised the results of one of us (Common 1985) to properties of states bound by potentials belonging to the two sets defined in § 3. Some of the constraints which have been obtained are very tight as are, for example, the energy bounds given in § 4 in the case of the linear potential.

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Appendix 1

We prove here the inequality (3.6a) for excited states. Let $z = z_i$ and $z = z_{i+1}$ be two adjacent zeros of the wavefunction $w_{n,l}(z)$ corresponding to energy $E(n, l)$ of the original system. Then $w_{n,l}(z)$ is the wavefunction for the *ground* state corresponding to the potential

$$\tilde{U}(z) = U(z)\theta(z-z_i)\theta(z_{i+1}-z). \tag{A1.1}$$

For fixed $z \geq 0$,

$$\tilde{U}(z) = \lim_{k\to\infty} \tilde{U}_k(z) \tag{A1.2}$$

where

$$\tilde{U}_k(z) = \left(\frac{z_i}{z}\right)^k + \left(\frac{z}{z_{i+1}}\right)^k + U(z). \tag{A1.3}$$

If $U(z)$ has positive Laplacian so do all the $\tilde{U}_k(z)$ for $k > 1$. For each k the ground-state wavefunction satisfies an inequality corresponding to (1.1) and for $z_i < z < z_{i+1}$, these wavefunctions will tend to $w_{n,\lambda}(z)$ which is the ground-state wavefunction for $\tilde{U}(z)$ as stated above. Therefore, for $z_i < z < z_{i+1}$,

$$-\left(\frac{w_{n,\lambda}(z)'}{w_{n,\lambda}(z)}\right)' \geq \frac{\lambda+1}{z^2} \qquad n, l = 0, 1, 2, \ldots. \tag{A1.4}$$

Using the methods of Common (1985) it then follows that

$$\int_{z_i}^{z_{i+1}} (w'_{n,\lambda}(z))^2\,dz \geqslant \frac{(\lambda+1)}{2}\int_{z_i}^{z_{i+1}} \frac{w^2_{n,\lambda}(z)}{z^2}\,dz. \tag{A1.5}$$

Repeating the argument for all the intervals between adjacent zeros of $w_{n,\lambda}(z)$ we obtain the inequality

$$\int_0^\infty (w'_{n,\lambda}(z))^2\,dz \geqslant \frac{(\lambda+1)}{2}\int_0^\infty \frac{w^2_{n,\lambda}(z)}{z^2}\,dz \tag{A1.6}$$

which is sufficient to prove (3.6a) since

$$\mathbb{T}_{n,\lambda} = \left(\int_0^\infty (w'_{n,\lambda}(z))^2\,dz + \lambda(\lambda+1)\int_0^\infty \frac{w^2_{n,\lambda}(z)}{z^2}\,dz\right)(\{1\}_{n,\lambda})^{-1}. \tag{A1.7}$$

Appendix 2

Since $u'_{0,l}(r)$ is positive (negative) for r less (greater) than r_{Ml}

$$\int_0^\infty u^2_{0,l}(r)\left(\frac{s+\alpha-1}{r^{s+\alpha}} - \frac{s-1}{r^2 r^\alpha_{Ml}}\right) dr$$

$$= 2\int_0^\infty u_{0,l}(r)u'_{0,l}(r)\left(\frac{1}{r^{s+\alpha-1}} - \frac{1}{r^{s-1}r^\alpha_{Ml}}\right) dr > 0 \tag{A2.1}$$

so long as s is such that all the integrals concerned exist. Therefore

$$r^\alpha_{Ml} \geqslant \left(\frac{s-1}{s+\alpha-1}\right)\frac{\langle r^{-s}\rangle_{0,l}}{\langle r^{-(s+\alpha)}\rangle_{0,l}}. \tag{A2.2}$$

Now

$$\frac{\langle r^{-s}\rangle_{0,l}}{\langle r^{-(s+\alpha)}\rangle_{0,l}} > \frac{\langle r^\alpha\rangle_{0,l}}{\langle 1\rangle_{0,l}}\frac{(2l+3-\alpha-s)}{(2l+3)} \tag{A2.3}$$

from (3.3) with $-s = 2(\alpha-1)+k\alpha$, $\alpha = 2(\alpha-1)+n\alpha$. Combining (A2.2) for $s>1$ and (A2.3)

$$r_{Ml} > \left(\frac{(s-1)(2l+3-\alpha-s)}{(s+\alpha-1)(2l+3)}\right)^{1/\alpha}\langle r\rangle_{0,l} \tag{A2.4}$$

since

$$\langle r^\alpha\rangle_{0,l} \geqslant \langle r\rangle^\alpha_{0,l} \qquad \text{for} \qquad \alpha > 1 \text{ as } \langle 1\rangle_{0,l} = 1.$$

The best bound is obtained by taking the value s which gives the maximum of the RHS of (A2.4).

The LHS of (5.1) is obtained by considering

$$\int_0^\infty u^2_{0,l}(r)[r^{s+\alpha}(s+\alpha+1) - r^s r^\alpha_{Ml}(s+1)]\,dr$$

$$= -2\int_0^\infty u_{0,l}(r)u'_{0,l}(r)(r^{s+\alpha+1} - r^{s+1}r^\alpha_{Ml})\,dr > 0. \tag{A2.5}$$

Therefore

$$r_{Ml} < \left(\frac{(s+\alpha+1)\langle r^{s+\alpha} \rangle_{0,l}}{(s+1)\langle r^{s} \rangle_{0,l}} \right)^{1/\alpha}.$$

Using (3.3) with $s = \alpha - 2 + n\alpha$ and $0 = 2(\alpha - 1) + k\alpha$

$$\frac{\langle r^{s+\alpha} \rangle_{0,l}}{\langle r^{s} \rangle_{0,l}} < \frac{\langle 1 \rangle_{0,l}(2l+s+3)}{\langle r^{-\alpha} \rangle_{0,l}(2l+3-\alpha)} \tag{A2.6}$$

and it follows from the inequality

$$\langle r^{-\alpha} \rangle_{0,l} \geqslant (\langle r \rangle_{0,l})^{-\alpha} \qquad \alpha > 1$$

that

$$r_{Ml} < \left(\frac{(s+\alpha+1)(2l+s+3)}{(s+1)(2l-\alpha+3)} \right)^{1/\alpha} \langle r \rangle_{0,l} \tag{A2.7}$$

which again can be optimised with respect to *s*.

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