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Properties of states bound by potentials with positive Laplacian

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Abstract. States of two-body systems bound by a spherically symmetric potential whose Laplacian is positive are considered. Constraints are derived on the kinetic energies and radii of states with the lowest energy for a given angular momentum, which improve on previous results of the author. These constraints become relatively very tight at high angular momentum. Inequalities are also derived between the energies of states of differing angular momentum and particle mass.

1. Introduction

In an earlier work (Common 1983) the properties of heavy quark-antiquark states were investigated in a potential model framework, and as such these are true for any two-body system bound by certain classes of spherically symmetric potentials. Recently Baumgartner *et al* (1984) have shown that the sign of the Laplacian of the potential, if it remains unchanged, determines the relative ordering of energy levels with the same principal Coulomb quantum number. They gave examples in nuclear, atomic and solid-state physics as well as particle physics where their results would hold.

Here the case when the Laplacian is positive is considered so that for a symmetric potential $V(r)$

$$\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}V(r)}{\mathrm{d}r}\right)>0 \qquad r>0. \tag{1.1a}$$

It is also assumed that

$$\lim_{r\to 0}(r^2V(r))=0. \tag{1.1b}$$

Baumgartner *et al* (1984) were then able to prove that

$$E(N,l)>E(N,l+1) \tag{1.2}$$

where $E(N,l)$ is the energy of the level with angular momentum l and principal Coulomb quantum number $N=n+l+1$, n being the number of nodes of the radial wavefunction. A crucial result in their proof was that for the class of potentials given in (1.1)

$$-\left(\frac{u_l'(r)}{u_l(r)}\right)'>\frac{l+1}{r^2} \tag{1.3}$$

where $u_l(r)$ is the reduced wavefunction of the ground state ($n=0$) corresponding to angular momentum l. In § 2 this result is used to obtain inequalities between average values of powers of r for given l and also bounds on $\int_0^\infty u_l'^2(r)\,dr$. It will be seen that the former take the form of 'reverse' Schwartz inequalities and may be used to bound the position and width of the peak of these ground states.

In § 3 upper and lower bounds to the kinetic energy of the above states are derived, which differ only by a numerical factor which tends to unity as $l\to\infty$. They therefore become relatively very tight for large l. Inequalities between energies of states of differing mass and angular momentum are also established, which in the framework of quarkonium models may be used to estimate mass differences between quarks of different types (Grosse and Martin 1978). In the final section the results and conclusions are presented.

2. The basic inequalities

The main inequalities used here are given by the following theorem, the proof of which is given in appendix 1.

Theorem. Let $u_l(r)$ be the ground-state wavefunction of angular momentum l corresponding to potential $V(r)$ satisfying (1.1). Then:

(i) if $n>k$ and are such that all integrals concerned exist

$$(l_1+l_2+2+k)\langle r^{k-1}\rangle_{l_1,l_2}\langle r^n\rangle_{l_1,l_2}\leqslant(l_1+l_2+2+n)\langle r^{n-1}\rangle_{l_1,l_2}\langle r^k\rangle_{l_1,l_2} \tag{2.1}$$

for all l_1, $l_2\geqslant 0$, where $\langle r^t\rangle_{l_1,l_2}\equiv\int_0^\infty r^t u_{l_1}(r)u_{l_2}(r)\,dr$;

(ii) for all $l\geqslant 0$

$$\int_0^\infty u_l'^2(r)\,dr\geqslant\frac{(l+1)}{2}\langle r^{-2}\rangle_l. \tag{2.2}$$

It is assumed that the $u_l(r)$, which have no nodes in $(0,\infty)$, are positive. The allowed values of n, k are determined by the behaviour $u_l(r)\simeq r^{l+1}$ as $r\to 0$ for potentials satisfying (1.1*b*).

The relations (2.1) are the reverse of the usual 'moment inequalities' as can be seen from the case with $l_1=l_2=l$; $k=1$, $n=2$. Then

$$\langle r^2\rangle_l\leqslant\left(\frac{2l+4}{2l+3}\right)\langle r\rangle_l^2 \tag{2.3}$$

which may be compared with the standard inequalities

$$\langle r^2\rangle_l\geqslant\langle r\rangle_l^2 \tag{2.4a}$$

in the general case, or (Common 1981)

$$\langle r^2\rangle_l\geqslant\frac{(4+2l)^2\langle r\rangle_l^2}{(3+2l)(5+2l)} \tag{2.4b}$$

when $dV/dr\geqslant 0$ for all $r>0$. The bounds are quite tight especially for this latter class of potentials. Even in the worst case ($l=0$) upper and lower bounds are in the ratio 5:4 while as $l\to\infty$ this ratio tends to unity. Bounds on the width of the peak $\Delta_l=(\langle r^2\rangle_l-\langle r\rangle_l^2)^{1/2}$ of the ground state of angular momentum l follow immediately from (2.3) and (2.4b) and are

$$\frac{1}{(2l+4)}\langle r^2\rangle_l^{1/2} \leqslant \Delta_l \leqslant \left(\frac{1}{2l+4}\right)^{1/2}\langle r^2\rangle_l^{1/2}. \tag{2.5}$$

These improve on the upper bounds given previously (Common 1983) especially for higher values of l. It must be remembered that the upper bounds (2.3), (2.5) are for the case when $V(r)$ has a *positive Laplacian.*

In this earlier work an upper bound was also obtained to the position $r = r_{Ml}$ of the maximum of $u_l^2(r)$ which is

$$r_{Ml} \leqslant 3^{1/2}\langle r^2\rangle_l^{1/2} \tag{2.6}$$

for all potentials. A corresponding lower bound was given in the case $l=0$ but not for other values. We now rectify this by using (2.1) with $l_1 = l_2 = l$; $n=1$, $k = -(2l+2)^{1/2}$ to prove in appendix 1 that

$$r_{Ml} \geqslant \langle r\rangle_l \times \begin{cases} [1-2(2l+2)^{1/2}/(2l+3)] & l > \frac{1}{4}(\sqrt{5}-1) \\ 2l/[(2l+1)(2l+3)] & 0 \leqslant l \leqslant \frac{1}{4}(\sqrt{5}-1). \end{cases} \tag{2.7}$$

The upper and lower bounds given by (2.6) and (2.7) are rather weak at low l, but their ratio tends to $\sqrt{3}:1$ as $l \to \infty$ so in this limit they are quite restrictive.

3. Bounds on the kinetic energy

In an earlier work (Common 1981) it was shown that the kinetic energy T_l of a state of angular momentum l has the upper bounds

$$T_l \leqslant \begin{cases} \frac{1}{2}\left\langle \frac{\mathrm{d}V}{\mathrm{d}r}\right\rangle_l \langle r\rangle_l & \text{if } \frac{\mathrm{d}^2V}{\mathrm{d}r^2} \leqslant 0 \quad r>0 & (3.1a) \\ \frac{1}{2}\left\langle \frac{\mathrm{d}V}{\mathrm{d}r}\right\rangle_l \frac{\langle r^2\rangle_l}{\langle r\rangle_l} & \text{if } \frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{1}{r}\frac{\mathrm{d}V}{\mathrm{d}r}\right) < 0 \quad r>0 & (3.1b) \end{cases}$$

and lower bounds

$$T_l \geqslant \frac{1}{2}\left\langle \frac{\mathrm{d}V}{\mathrm{d}r}\right\rangle_l \frac{\langle r^{-1}\rangle_l}{\langle r^{-2}\rangle_l} \tag{3.1c}$$

if $V(r)$ satisfies (1.1). Using (2.1) the following inequalities are easily derived:

$$R_l \times \frac{1}{2}\left\langle \frac{\mathrm{d}V}{\mathrm{d}r}\right\rangle_l \langle r\rangle_l \leqslant T_l \leqslant \frac{1}{2}\left\langle \frac{\mathrm{d}V}{\mathrm{d}r}\right\rangle_l \langle r\rangle_l \tag{3.2a}$$

and

$$\frac{1}{2}\left\langle \frac{\mathrm{d}V}{\mathrm{d}r}\right\rangle_l \frac{\langle r^{-1}\rangle_l}{\langle r^{-2}\rangle_l} \leqslant T_l \leqslant \frac{1}{2}\left\langle \frac{\mathrm{d}V}{\mathrm{d}r}\right\rangle_l \frac{\langle r^{-1}\rangle_l}{\langle r^{-2}\rangle_l} R_l^{-1} \tag{3.2b}$$

where $R_l = (2l+1)/(2l+3)$ and $(2l+1)/(2l+4)$ for the two classes of potentials corresponding to (3.1a) and (3.1b) respectively. These relations have the nice feature that upper and lower bounds differ only by a numerical factor which tends to unity as $l \to \infty$. The bounds are particularly useful in the case when $l=0$ for then $\langle \mathrm{d}V/\mathrm{d}r\rangle_l = (1/m)|u_s'(0)|^2$ where m is the mass of each of the identical particles in the bound system. They were used (Common 1981) to obtain bounds on quark mass differences from the leptonic decay roles of quarkonium states which give estimates for $|u_s'(0)|^2$.

Alternative bounds to T_l may be obtained in terms of $\langle 1/r^2\rangle_l$ and these results lead to relations between energy levels of states of different particle mass and angular momentum as will be shown later. A lower bound follows immediately from (2.2):

$$T_l = \frac{1}{m}\int_0^\infty \left(u_l'^2 + \frac{l(l+1)}{r^2}u_l^2\right) \mathrm{d}r \geqslant \frac{1}{m}(l+1)(l+\tfrac{1}{2})\langle r^{-2}\rangle_l \tag{3.3}$$

for potentials satisfying (1.1). This improves on our previous bound (Common 1983) obtained for potentials such that $(\mathrm{d}/\mathrm{d}r)^3(r^2V(r)) \geqslant 0$ and $-\infty < \lim_{r\to 0}(rV(r)) \leqslant 0$, the latter in particular being a *more* restrictive condition compared with (1.1).

For this class of potentials, Grosse and Martin (1978) have obtained the inequality

$$E(M_1, (M_1/M_0)^{1/2} - 1) \leqslant E(M_0, 0) \qquad M_1 > M_0 > 0 \tag{3.4}$$

for energy levels $E(m, l)$ of the bound states with angular momentum l of identical particles of mass m. We now recover this bound for our alternative class of potentials with positive Laplacian.

We have that

$$\frac{\partial E(m,l)}{\partial m} = -\frac{T_l}{m} \qquad \frac{\partial E(m,l)}{\partial l} = (2l+1)\langle r^{-2}\rangle_l \tag{3.5}$$

and using (3.3), that

$$\frac{\partial E}{\partial l}\left(\frac{l+1}{2}\right) + m\frac{\partial E}{\partial m} \leqslant 0. \tag{3.6}$$

Setting $2\ln(l+1) = \ln m/M_0 \equiv \lambda$ and integrating (3.6) from $\lambda = 0$ to $\lambda = \ln M_1/M_0$, we do in fact obtain the bound (3.4). The method can be easily generalised to the case when $l \neq 0$ on the RHS.

A *new* complementary upper bound for the kinetic energy when $l > \frac{1}{2}$ is given by

$$T_l \leqslant (W_l/m)\langle r^{-2}\rangle_l \tag{3.7}$$

where $W_l = (l+1)(l+\frac{3}{2})$ and $(l+1)(l+2)$ for the potentials of inequalities (3.1a) and (3.1b) respectively. For angular momenta $0 \leqslant l \leqslant \frac{1}{2}$ we have to make the added assumption that $\mathrm{d}V/\mathrm{d}r \geqslant 0$ for all $r > 0$, and then the bound (3.7) holds with $W_l = \frac{15}{4} - l(l+1)$ and $\frac{9}{2} - l(l+1)$ respectively. The proofs are given in appendix 2.

Corresponding to (3.6), we have for monotonic increasing concave potentials satisfying (1.1) that

$$\begin{aligned} &\frac{[\frac{15}{4} - l(l+1)]}{(2l+1)}\frac{\partial E(m,l)}{\partial l} + m\frac{\partial E(m,l)}{\partial m} \geqslant 0 \qquad && \tfrac{1}{2} \geqslant l \geqslant 0 \\ &\frac{(l+1)(l+\frac{3}{2})}{(2l+1)}\frac{\partial E(m,l)}{\partial l} + m\frac{\partial E(m,l)}{\partial m} \geqslant 0 \qquad && l > \tfrac{1}{2}. \end{aligned} \tag{3.8}$$

Proceeding as above we take

$$\lambda = \ln\frac{m}{M_0} = \int_0^l F(l')\,\mathrm{d}l' \tag{3.9}$$

where

$$F(l)=\begin{cases}(2l+1)/[\frac{15}{4}-l(l+1)] & \frac{1}{2}\geq l\geq 0, \quad (3.10a)\\ (2l+1)/[(l+1)(l+\frac{3}{2})] & l>\frac{1}{2}. \quad (3.10b)\end{cases}$$

Then (3.8) is equivalent to the relation $\mathrm{d}E/\mathrm{d}\lambda\geq 0$. Integrating this inequality from $\lambda=0$ to $\lambda=\ln M_1/M_0$

$$E(M_1, L_1)\geq E(M_0, 0) \qquad M_1>M_0>0 \tag{3.11}$$

where L_1 is the positive root of

$$l^2+l-\tfrac{15}{4}(1-M_0/M_1)=0 \tag{3.12a}$$

if this root is $\leq\frac{1}{2}$ and otherwise is the positive root of

$$l^2+\left[3-\frac{16}{3\sqrt{5}}\left(\frac{M_1}{M_0}\right)^{1/2}\right]l+\frac{9}{4}-\frac{16}{3\sqrt{5}}\left(\frac{M_1}{M_0}\right)^{1/2}=0. \tag{3.12b}$$

Similar bounds may be obtained for the class of potentials of (3.1b) and they complement the lower bounds to $E(M_0, 0)$ given by (3.4).

4. Summary and conclusions

For the class of potentials with positive Laplacian, inequalities have been derived between average values of powers of the interparticle distance of the corresponding two-particle ground states of given angular momentum l. They are the reverse of the usual 'moment' inequalities and lead to upper and lower bounds on physical quantities which have the nice feature of differing only by a numerical factor. Also this factor tends to unity as $l\to\infty$ so these bounds become relatively very tight at large l.

In the past constraints of the type discussed here have been used in the framework of potential models of quarkonium. For instance, bounds were put on the difference between the masses of the 'charmed' and 'bottom' quarks (Martin and Grosse 1978, Common 1981) and on the masses of 'beautiful' hadrons (Martin 1981). With some assumptions on the spin nature of the quark-antiquark forces, Khare (1981a) studied the fine structure of the quarkonium spectroscopy using the above type of bounds and he also obtained bounds on the decay rates of some of these states, (Khare 1981b). The new bounds discussed here could lead to further developments in this field of study.

Appendix 1

Proof of (2.1) and (2.2). Consider

$$\begin{aligned} I_{l_1,l_2}&\equiv\int_0^\infty\frac{1}{r^2}\int_0^r u_{l_1}(r')u_{l_2}(r')(r'^k\langle r^n\rangle_{l_1,l_2}-r'^n\langle r^k\rangle_{l_1,l_2})\,\mathrm{d}r'\,\mathrm{d}r\\ &=\int_0^\infty u_{l_1}(r)u_{l_2}(r)(r^{k-1}\langle r^n\rangle_{l_1,l_2}-r^{n-1}\langle r^k\rangle_{l_1,l_2})\,\mathrm{d}r\\ &=\langle r^{k-1}\rangle_{l_1,l_2}\langle r^n\rangle_{l_1,l_2}-\langle r^{n-1}\rangle_{l_1,l_2}\langle r^k\rangle_{l_1,l_2}. \end{aligned}\tag{A1.1}$$

If phases are chosen so that $u_l(r) \geqslant 0$ for all $r \geqslant 0$, then

$$\int_0^r u_{l_1}(r')u_{l_2}(r')(r'^k\langle r^n\rangle_{l_1,l_2} - r'^n\langle r^k\rangle_{l_1,l_2})\,\mathrm{d}r'$$

is positive for all $r > 0$ when $k < n$, since the integrand changes sign only once, being positive close to $r = 0$ while the integral $\to 0$ as $r \to \infty$. using (1.3) we find

$$\begin{aligned}[(l_1+1)+(l_2+1)]I_{l_1,l_2} &\leqslant -\sum_{i=1}^{2}\int_0^\infty \left(\frac{u'_{li}}{u_{li}}\right)'\int_0^r u_{l_1}(r')u_{l_2}(r')(r'^k\langle r^n\rangle_{l_1,l_2} - r'^n\langle r^k\rangle_{l_1,l_2})\,\mathrm{d}r'\,\mathrm{d}r \\ &= -k\langle r^{k-1}\rangle_{l_1,l_2}\langle r^n\rangle_{l_1,l_2} + n\langle r^{n-1}\rangle_{l_1,l_2}\langle r^k\rangle_{l_1,l_2} \qquad \text{(A1.2)}\end{aligned}$$

on integrating by parts twice. This result is equivalent to (2.1).

Similarly,

$$\frac{(l+1)}{2}\int_0^\infty \frac{u_l^2(r)}{r^2}\,\mathrm{d}r \leqslant -\frac{1}{2}\int_0^\infty \left(\frac{u'_l}{u_l}\right)' u_l^2(r)\,\mathrm{d}r = \int_0^\infty u_l'^2\,\mathrm{d}r \qquad \text{(A1.3)}$$

is equivalent to (2.2).

To obtain lower bounds to r_{Ml}, we use the fact that

$$\int_0^\infty u_l^2\left(\frac{s}{r^{s+1}} - \frac{s-1}{r^s r_{Ml}}\right)\mathrm{d}r = 2\int_0^\infty \frac{u_l u'_l}{r^s r_{Ml}}(r_{Ml} - r)\,\mathrm{d}r \geqslant 0 \qquad \text{(A1.4)}$$

so long as the integrals exist which require $s < 2l+1$. Therefore for these values of s

$$r_{Ml} \geqslant \frac{(s-1)}{s}\frac{\langle r^{-s}\rangle_l}{\langle r^{-s-1}\rangle_l} \geqslant \left(\frac{s-1}{s}\right)\left(\frac{2l+2-s}{2l+3}\right)\langle r\rangle_l \qquad \text{(A1.5)}$$

from (2.1) with $n = 1$, $k = -s$ and $l_1 = l_2 = l$. The bound (2.7) is the maximum of the right-hand side of (A1.5) as a function of $s < 2l+1$.

Appendix 2

For the class of potentials in (3.1*a*)

$$\begin{aligned} T_l &\leqslant \tfrac{1}{2}\langle r\rangle_l \int_0^\infty u_l^2 \frac{\mathrm{d}V}{\mathrm{d}r}\,\mathrm{d}r \\ &= \frac{l(l+1)}{m}\langle r\rangle_l\langle r^{-3}\rangle_l \qquad l > \tfrac{1}{2} \qquad \text{(A2.1)} \\ &\leqslant \frac{(l+1)(l+\frac{3}{2})}{m}\langle r^{-2}\rangle_l \end{aligned}$$

on using (2.1). The corresponding result for the potentials (3.1*b*) follows in the same manner and may be continued to $l = \frac{1}{2}$.

For $0 \leqslant l < \frac{1}{2}$ we have to work a little harder. We use an approach developed by Bertlmann and Martin (1980) to bound $\partial T_l/\partial m$ by $-\partial E(m, l)/\partial m$. Now $\partial u_l(r)/\partial l$ has a unique zero in $(0, \infty)$ say at $r = r_0$. To prove this we use the method of Rosner *et al*

(1978). The radial equation for $u_l(r)$ is taken in the form

$$u_l''(r)/u_l(r)=m(V(r)-E(m,l))+l(l+1)/r^2. \tag{A2.2}$$

Differentiating with respect to l, multiplying by u_l^2 and integrating over $(0, r)$ gives

$$u_l^2\frac{\mathrm{d}}{\mathrm{d}r}\left(u_l^{-1}\frac{\partial u_l}{\partial l}\right)=(u_l(r)\,\partial u_l'/\partial l-u_l'\,\partial u_l/\partial l)$$

$$=m\int_0^r\left(-\frac{\partial E_l}{\partial l}+\frac{(2l+1)}{mr'^2}\right)u_l(r')^2\,\mathrm{d}r'\geqslant 0. \tag{A2.3}$$

The last inequality follows from the fact that the integrand has only one zero in $(0,\infty)$, is positive close to $r=0$ and as $r\to\infty$ the integral $\to 0$ from (3.5). Therefore $u_l^{-1}\,\partial u_l/\partial l$ is an increasing function of r and has exactly one zero since $\int_0^\infty u_l\,\partial u_l/\partial l\,\mathrm{d}r=0$. Then using the 'virial theorem',

$$\frac{\partial T_l}{\partial l}=\int_0^\infty u_l\frac{\partial u_l}{\partial l}(rV'(r)-r_0V'(r_0))\,\mathrm{d}r \tag{A2.4}$$

and

$$\frac{\partial E(m,l)}{\partial l}=\int_0^\infty u_l\frac{\partial u_l}{\partial l}\left(V(r)+\frac{r}{2}V'(r)-V(r_0)-\frac{r_0}{2}V'(r_0)\right)\mathrm{d}r. \tag{A2.5}$$

For the class of potentials with positive Laplacian, the right-hand side of (A2.5) is positive since $\partial u_l/\partial l$ is <0 for r close to zero. Hence

$$\left(\frac{\partial T_l}{\partial E}\right)\left(\frac{\partial E}{\partial l}\right)^{-1}\geqslant\inf\left(\frac{(\mathrm{d}/\mathrm{d}r)(\frac{1}{2}r\,\mathrm{d}V/\mathrm{d}r)}{(\mathrm{d}/\mathrm{d}r)(V(r)+\frac{1}{2}r\,\mathrm{d}V/\mathrm{d}r)}\right)=-1 \tag{A2.6}$$

when $\mathrm{d}V/\mathrm{d}r\geqslant 0$ all r, so that

$$T_l\leqslant T_{1/2}+\int_l^{1/2}\frac{\partial E(l',m)}{\partial l'}\,\mathrm{d}l'=T_{1/2}+\int_l^{1/2}(2l'+1)\langle r^{-2}\rangle_{l'}\,\mathrm{d}l'. \tag{A2.7}$$

However, again from the fact (Common 1980) that $u_{l'}^2-u_l^2$ has a unique zero in $(0,\infty)$, $\langle r^{-2}\rangle_{l'}\leqslant\langle r^{-2}\rangle_l$ for $l\leqslant l'$. So finally for $0\leqslant l\leqslant\frac{1}{2}$

$$T_l\leqslant T_{1/2}+\int_l^{1/2}(2l'+1)\,\mathrm{d}l'\langle r^{-2}\rangle_l$$

$$=T_{1/2}+[\tfrac{3}{4}-l(l+1)]\langle r^{-2}\rangle_l. \tag{A2.8}$$

Using the bounds (A2.1) for $T_{1/2}$ we arrive at our result.

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