CERN-TH-5843/90

**SPACINGS OF PURELY ANGULAR EXCITATIONS IN POTENTIALS
WITH A LAPLACIAN OF A GIVEN SIGN, AND APPLICATIONS**

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ABSTRACT

Purely angular excitations of two-body systems with a spherically symmetric interacting potential whose Laplacian has definite sign are considered. It is shown that the ratio of level spacings between different angular momenta is bounded below (above) by the ratio of the corresponding spacings for the Coulomb problem when the Laplacian of the potential is positive (negative). These estimates are applied to quarkonium models, muonic atoms, alkaline atoms, and exponentially screened Coulomb potentials.

CERN-TH-5843/90

August 1990

1. Introduction and main result

In 1984, Baumgartner, Grosse and Martin (BGM) [1] proved that if, in the two-body Schrödinger equation, the interacting potential is spherically symmetric and has a Laplacian with a given sign, the order of levels corresponding to what would be a degenerate multiplet for the Coulomb potential is known. Specifically the Coulomb-multiplet is characterized by $N = \ell + n + 1$, ℓ being the angular momentum and n the number of nodes of the radial wave function. Then if $\Delta V(r) > 0$, the energies decrease when ℓ increases (keeping N fixed), and if $\Delta V(r) < 0$ the energies increase when ℓ increases. The key to this result is an inequality for the ground states with angular momentum ℓ :

$$\text{If } \Delta V(r) \gtrless 0 \text{ for } r > 0, \quad -\left(\frac{u_\ell'}{u_\ell}\right)' - \frac{\ell+1}{r^2} \gtrless 0 \quad (1.1)$$

for $r > 0$ (BGM inequality). Here u_ℓ is the reduced ground state wave function with angular momentum ℓ , i.e., u_ℓ solves the reduced Schrödinger equation

$$-u_\ell'' + \frac{\ell(\ell+1)}{r^2}u_\ell + V(r)u_\ell - E_\ell u_\ell = 0 \quad (1.2)$$

and $u_\ell(r) > 0$ for $r > 0$. Here E_ℓ is the ground state energy. In other words, as noticed by Asbaugh and Benguria [2], the BGM-inequality says that

$$\log \frac{u_\ell}{r^{\ell+1}} \text{ is } \begin{matrix} \text{concave} \\ \text{convex} \end{matrix} \text{ if } \Delta V \gtrless 0$$

Recently, a rather simple proof of the BGM-inequality was given by Martin [3]. Common [4] discovered that the BGM-inequality leads to interesting inequalities on the moments

$$\langle r^\nu \rangle_\ell \equiv \int_0^\infty r^\nu u_\ell^2(r) dr. \quad (1.3)$$

Common and Martin [5,6] derived concavity properties of the ground state energies E_ℓ considered as a function of the angular momentum ℓ . In particular they obtained the following

inequality for ground state energies of potentials with negative Laplacian [6].

$$\frac{E_{\ell+1} - E_\ell}{E_\ell - E_{\ell-1}} \leq \frac{\ell}{\ell+2} \quad (1.4)$$

However, the above inequality is not optimal in the sense that it is not saturated for the ground state energies of the Coulomb problem. In fact, it is conjectured that the constant in the right-hand side of (1.4) is given by the ratio of the corresponding Coulomb energies [6]. Secondly, no inequality for potentials with positive Laplacian of the form (1.4) is known up to now. In this letter we remedy these deficiencies and prove the following result.

Theorem:

If $\Delta V \gtrless 0$, then for any triple (k, ℓ, m) with $0 \leq k < \ell < m$

$$\frac{E_m - E_\ell}{E_\ell - E_k} \gtrless \frac{E_m - E_k}{E_\ell - E_k}$$

where $E_\ell^c = -\frac{1}{4(\ell+1)^2}$ denotes the ground state energy with angular momentum ℓ for the Coulomb problem (i.e., $V(r) = -\frac{1}{r}$). In particular, for the ratio of neighbored gaps, one has

$$\frac{E_{\ell+1} - E_\ell}{E_\ell - E_{\ell-1}} \gtrless \frac{2\ell+3}{2\ell+1} \left(\frac{\ell}{\ell+2}\right)^2$$

The energy differences may be viewed as transition energies (or mass gaps) and therefore the quality of our result can be checked by experimental or numerical values obtained for two-body systems with a spherically symmetric interacting potential whose Laplacian has a definite sign. We shall apply the estimates of the theorem to quarkonium models, X-ray transitions in muonic atoms, alkaline atoms, and energy levels of an exponentially screened Coulomb potential.

In potential models of quarkonium the potential is supposed to be derived from QCD. The force between a quark-antiquark pair can be written as

$$\frac{\alpha(r)}{r^2}$$

In the Coulomb case $\alpha(r)$ would be constant but because of asymptotic freedom, $\alpha(r)$ is an

increasing function of r . In terms of the potential this means that

$$\frac{d}{dr} r^2 \frac{dV}{dr} > 0$$

i.e., that the Laplacian of the potential is positive for all $r > 0$. In fact, all existing phenomenological potentials satisfy this condition.

Muonic atoms are also a good testing ground for inequalities on potentials with positive Laplacian. In fact, in muonic atoms the nucleus (of charge Z) cannot be anymore considered as pointlike because the radius of the Bohr orbits is 200 Z times smaller than that of ordinary hydrogen, while the radius of the nucleus increases like $Z^{1/3}$. The potential is produced by a positive charge distribution and by Gauss' law it has a positive Laplacian.

On the other hand, alkaline atoms give an example of a potential with negative Laplacian if one accepts to believe the Hartree approximation: the potential acting on the outer electron is produced by the nucleus which in this situation can be regarded as pointlike and the negatively charged electron cloud of the filled shells. Equally the exponentially screened Coulomb potential

$$V(r) = -\frac{Ze^2}{r} \exp(-r/D)$$

which provides an approximate representation of many-body effects in a plasma has a negative Laplacian. Here, D is the screening length (in plasma theory called Debye screening length). The range of the potential is of the order of D .

In a forthcoming paper we shall extend the results of this letter and obtain sharp inequalities on moments, kinetic energies and potential energies of reduced ground states.

2. Proof of the main result

To prove the theorem we consider the angular momentum ℓ as a continuous rather than a discrete variable. We show the following theorem.

Theorem 2.1

If $\Delta V \geq 0$, then E_ℓ satisfies the differential inequality

$$\frac{\partial^2 E_\ell}{\partial \ell^2} < -\frac{3}{\ell+1} \frac{\partial E_\ell}{\partial \ell}$$

The inequality is sharp and saturated by the ground state eigenvalues of the Coulomb problem.

The estimate on the eigenvalue gaps follows then by integrating twice the differential inequality of Theorem 2.1.

Essentially we use two tools to prove our result. The first one is the BGM-inequality, the second is the following basic integral inequality, which is due to Tchebychev (see, e.g., [7], Theorem 236).

Lemma 2.2: Let $f, g, h, \mathbf{R}_0^+ \rightarrow \mathbf{R}$ such that f and g are non-decreasing (or non-increasing) and h is non-negative. Then

$$\int_0^\infty f h dx \int_0^\infty g h dx \leq \int_0^\infty f g h dx \int_0^\infty h dx$$

As a first consequence of these two inequalities we prove a generalization of Commott's moment inequalities.

Proposition 2.3: Let $A, B : \mathbf{R}_0^+ \rightarrow \mathbf{R}$ be functions such that A is non-decreasing and B is non-negative. In addition, we assume that the functions $B(r)u_\ell^2(r)$ and $A(r)B(r)u_\ell^2(r)$ vanish at zero and at infinity where u_ℓ is the reduced ground state with angular momentum ℓ . By $\langle \cdot \rangle_\ell$ we denote the expectation values with respect to $u_\ell^2 dr$. If $\Delta V \geq 0$, then

$$\left\langle \left(AB' + \frac{2\ell+2}{r} AB \right) \right\rangle_\ell \geq \left\langle B' + \frac{2\ell+2}{r} B \right\rangle_\ell \langle AB \rangle_\ell$$

provided all integrals exist.

Proof of Proposition 2.3. We apply Lemma 2.2 choosing $f = -\text{sign}(\Delta V) \left(\frac{u_\ell}{u_\ell} - \frac{\ell+1}{r} \right)$, $g = A$ and $h = Bu_\ell^2$. Note that f is non-decreasing by the BGM-inequality. Integration by parts yields the desired result.

In particular, we need the following examples of Proposition 2.3.

Example 2.4: Let $A = r^\alpha$ and $B = r^\beta$ with $\alpha \geq 0$ and $\beta > -2\ell - 3$. Then

$$(2\ell + 2 + \alpha + \beta) \left\langle r^{\alpha+\beta-1} \right\rangle_\ell \left\langle r^\beta \right\rangle_\ell \geq (2\ell + 2 + \beta) \left\langle r^{\beta-1} \right\rangle_\ell \left\langle r^{\alpha+\beta} \right\rangle_\ell$$

depending on whether $\Delta V \geq 0$.

Example 2.5: Let $A = \ln r$ and $B = r^\beta$ with $\beta > -2\ell - 3$. If $\Delta V \geq 0$ we find the inequality

$$[(2\ell + 2 + \beta) \left\langle r^{\beta-1} \ln r \right\rangle_\ell + \left\langle r^{\beta-1} \right\rangle_\ell \left\langle r^\beta \right\rangle_\ell] \left\langle r^\beta \right\rangle_\ell \geq (2\ell + 2 + \beta) \left\langle r^{\beta-1} \right\rangle_\ell \left\langle r^\beta \ln r \right\rangle_\ell$$

Next we compute the derivatives of E_ℓ with respect to ℓ . It can be easily shown that the curve u_ℓ is differentiable with respect to ℓ , i.e.,

$$v_\ell \equiv \frac{\partial u_\ell}{\partial \ell} \quad (2.1)$$

exists. Then we have

$$\frac{\partial E_\ell}{\partial \ell} = (2\ell + 1) \int_0^1 \frac{1}{r^2} u_\ell^2 dr \quad (2.2)$$

by the Feynman-Hellmann relation and

$$\frac{\partial E_\ell}{\partial \ell} = 2 \int_0^1 \frac{1}{r^2} u_\ell^2 dr + 2(2\ell + 1) \int_0^1 \frac{1}{r^2} u_\ell v_\ell dr \quad (2.3)$$

In the sequel we make use of the following lemma about v_ℓ , which was proved in [6].

Lemma 2.6: The function v_ℓ/u_ℓ is increasing for $r > 0$. In particular, u_ℓ and v_ℓ satisfy the Wronskian relation

$$(v_\ell u_\ell - u_\ell' v_\ell)(r) = \int_0^r \left(\frac{2\ell + 1}{s^2} - \frac{\partial E_\ell}{\partial \ell} \right) u_\ell^2 ds \quad (2.4)$$

To prove Theorem 2.1 we only have to bound the second integral in (2.3) in terms of the moment $\langle r^2 \rangle_\ell$. In the following we work out the case $\Delta V < 0$. For $\Delta V > 0$ all inequalities to be used go in the opposite direction.

Integrating the second integral of (2.3) by parts twice and using (2.4) we compute

$$\begin{aligned} \int_0^\infty \frac{1}{r^2} u_\ell v_\ell dr &= \int_0^\infty \frac{1}{r} (u_\ell v_\ell)' dr \\ &= 2 \int_0^\infty \frac{1}{r} u_\ell v_\ell dr + \int_0^\infty \frac{1}{r} \left(\frac{2\ell + 1}{s^2} - \frac{\partial E_\ell}{\partial \ell} \right) u_\ell^2 ds dr \\ &= 2 \int_0^\infty \frac{1}{r} u_\ell v_\ell dr - \int_0^\infty \ln r \left(\frac{2\ell + 1}{r^2} - \frac{\partial E_\ell}{\partial \ell} \right) u_\ell^2 dr \end{aligned} \quad (2.5)$$

We estimate the first term of the last line in (2.5). Since $\frac{u_\ell}{u_\ell} - \frac{\ell+1}{r}$ is non-decreasing by the BGM-inequality and $\frac{u_\ell}{u_\ell}$ is non-decreasing by Lemma 2.6. We may apply Lemma 2.2 with $f = \frac{u_\ell}{u_\ell}$, $g = \frac{u_\ell}{u_\ell} - \frac{\ell+1}{r}$ and $h = \frac{1}{r} u_\ell^2$ to obtain

$$\int_0^\infty \frac{1}{r} u_\ell v_\ell dr - \int_0^\infty \left(\frac{1}{r} u_\ell' u_\ell - \frac{\ell+1}{r^2} u_\ell^2 \right) dr < \int_0^\infty \frac{1}{r} u_\ell^2 dr \int_0^\infty \left(\frac{1}{r} u_\ell' v_\ell - \frac{\ell+1}{r^2} u_\ell v_\ell \right) dr$$

Inserting the identity (2.5) for $\int_0^\infty \frac{1}{r} u_\ell v_\ell dr$ and simplifying, we arrive at the following inequality

$$\left[\int_0^\infty \frac{2\ell+1}{r^2} u_\ell v_\ell dr - \int_0^\infty \ln r \left(\frac{2\ell+1}{r^2} - \frac{\partial E_\ell}{\partial \ell} \right) u_\ell^2 dr \right] \int_0^\infty \frac{1}{r} u_\ell^2 dr < \int_0^\infty \frac{1}{r} u_\ell v_\ell dr \int_0^\infty \frac{2\ell+1}{r^2} u_\ell^2 dr \quad (2.6)$$

We estimate the first integral of the right-hand side of (2.6) as follows. Integration by parts yields $\int_0^\infty \frac{1}{r} u_\ell v_\ell dr = \int_0^\infty \frac{1}{r^2} \int_0^r u_\ell v_\ell ds dr$ since $\int_0^\infty u_\ell v_\ell dr = 0$. Now, $\int_0^r u_\ell v_\ell ds$ is negative for all

$r > 0$. Therefore, by the BGM-inequality we have

$$\begin{aligned} \int_0^1 \frac{1}{r} u_l v_l dr &< - \int_0^1 \frac{1}{\ell+1} \left(\frac{u_l'}{u_l} \right)' \int_0^r u_l v_l ds dr \\ &= \frac{1}{2\ell+2} \int_0^\infty (u_l' v_l - v_l' u_l) dr \quad (\text{by integration by parts}) \\ &= \frac{1}{2\ell+2} \int_0^\infty \frac{2\ell+1}{r} u_l^2 dr - \frac{1}{2\ell+2} \frac{\partial E_\ell}{\partial \ell} \int_0^\infty r u_l^2 dr \quad (\text{by (2.4)}) \end{aligned}$$

With help of this inequality and inequality (2.6) we find (expressing all integrals and $\frac{\partial E_\ell}{\partial \ell}$ as moments)

$$\frac{\partial^2 E_\ell}{\partial \ell^2} < 2 \langle r^{-2} \rangle_\ell + \frac{(2\ell+1)^2 \langle r^{-2} \rangle_\ell}{\ell+1} \left[\langle r^{-1} \rangle_\ell - \langle r \rangle_\ell \langle r^{-2} \rangle_\ell + 2(2\ell+1) \left\langle \frac{\ln r}{r^2} \right\rangle_\ell - \langle \ln r \rangle_\ell \langle r^{-2} \rangle_\ell \right] \quad (2.7)$$

Now, by the moment's inequalities, we have

$$(2\ell+1) \langle r^{-2} \rangle_\ell \langle r \rangle_\ell > (2\ell+3) \langle 1 \rangle_\ell \langle r^{-1} \rangle_\ell$$

(example 2.4 with $\alpha = 2$ and $\beta = -1$), and

$$\left[\left\langle \frac{\ln r}{r^2} \right\rangle_\ell - \langle \ln r \rangle_\ell \langle r^{-2} \rangle_\ell \right] < - \left[\frac{1}{2\ell+2} + \frac{1}{2\ell+1} \right] \langle r^{-2} \rangle_\ell$$

(example 2.5, combination of the cases $\beta = -1$ and $\beta = 0$). Therefore (2.7) implies

$$\frac{\partial^2 E_\ell}{\partial \ell^2} < \frac{2\ell+1}{\ell+1} (-2-1) \langle r^{-2} \rangle_\ell = - \frac{3}{\ell+1} \frac{\partial E_\ell}{\partial \ell}$$

and Theorem 2.1 is proved.

3. Applications

The first application is, as we said in the Introduction, to quarkonium, because the potential is expected to have a positive Laplacian. Indeed, if we consider the $c\bar{c}$ bound state system we have

$$M(n, 0, \ell = 0) = 3.07 \text{ GeV}/c^2 \quad (3.1a)$$

(weighted average between J/ψ and η_c),

$$M(n = 0, \ell + 1) = 3.52 \text{ GeV}/c^2 \quad (3.1b)$$

(weighted average on triplet p -state), and

$$M(n = 0, \ell = 2) = 3.77 \text{ GeV}/c^2 \quad (3.1c)$$

($j = 1$ d -state, other states being as yet unobserved).

Hence we get

$$\frac{E_2 - E_1}{E_1 - E_0} = 0.55 > 0.185 \quad (3.2)$$

As we see the inequality is too well satisfied. One more interesting example would be the upsilon which is a $b\bar{b}$ bound state. However, the d -states have not been observed so far but we can hope to see them as products of radiative decays of excited p -states [8].

The second application we present is to muonic atoms. We analyzed the values for X -ray transitions compiled by R. Engfer et al. [9] for three ratios of transition energies. For a detailed review about energy levels of muonic atoms we refer to [10]. The ratios obtained from the experimental data are shown in Fig. 1. However, these data cannot be used directly to test our inequality, since relativistic effects cannot be neglected (at least for large Z). Therefore we have to renormalize the measured data to values of the Schrödinger theory.

There we have used when available averages on transitions corresponding to various spin states. However, even for a point nucleus, we know that the Schrödinger equation should be replaced by the Dirac equation, especially for large Z . For Z not too large, an approximate formula for the binding energy is

$$B_D \simeq B_S \left[1 + \frac{(Z\alpha)^2}{N} \left(\frac{1}{J+1/2} - \frac{3}{4N} \right) \right] \quad (3.3)$$

where N is the principal quantum number, J the total angular momentum ($J+1/2 \leq N$) B_D is the "Dirac" binding energy and B_S the "Schrödinger" binding energy. Equation (3.3) suggests that by making a certain linear combination of the transition energies corresponding to the same initial and final N and orbital angular momentum, namely, $N = \ell + 1, \ell + 1 \rightarrow N = \ell, \ell$, but different spin states, one can eliminate the Dirac corrections. In fact we have done this, using the exact Dirac values, and adjusting the coefficients in such a way that the error remains small for $1 \leq Z \leq 82$. We found:

$$\begin{aligned} & |3.62(2p_{1/2} \rightarrow 1s_{1/2})D - 2.62(2p_{3/2} - 1s_{1/2})D - (2p - 1s)|s| < 8 \times 10^{-5} m_{\mu\text{on}} \\ & |1.18(3d_{5/2} - 2p_{3/2})D - 0.18(3d_{3/2} - 2p_{1/2})D - (3d - 2p)|s| < 2.6 \times 10^{-5} m \\ & |1.41(4f_{7/2} - 3d_{5/2})D - 0.41(4f_{5/2} - 3d_{3/2})D - (4f - 3d)|s| < 0.15 \times 10^{-5} m \\ & |1.62(5g_{9/2} - 4f_{7/2})D - 0.62(5g_{7/2} - 4f_{5/2})D - (5g - 3d)|s| < 0.4 \times 10^{-6} m \end{aligned}$$

(here the indices S and D refer to Schrödinger and Dirac).

So if we take these combinations, and if QED corrections such as vacuum polarization are small enough, which is the case [10], the ratios of the successive transitions should coincide with the Schrödinger prediction for the hydrogen atom. Deviations should be indicative of the effect of the finite size of the nucleus. This is what we have done in Fig. 2. We see that it is the $(3d - 2p)/(2p - 1s)$ ratio which is most sensitive to finite size effects as one could expect and deviates from the hydrogen ratio in the direction predicted by the theorem, more and more as Z increases. The finite size effect is still visible on the $(4f - 3d)/(3d - 2p)$ ratio, while the $(5g - 4f)/(4f - 3d)$ ratio is unaffected (here the Dirac to Schrödinger conversion is essential!).

Now, as we said in the Introduction, the outer electron of an alkaline atom is submitted, in the Hartree approximation, to a potential with negative Laplacian. In Fig. 3, we show the level diagram of the lithium atom, for which it happens that the $4f - 3d$ and $3d - 2p$ transitions are measured. The ratio $(4f - 3d)/(3d - 2p)$ is found to be 0.3264, i.e., less than 0.35 in agreement with our theorem.

Finally, our result is applied to numerically obtained eigenvalues of the exponentially screened Coulomb potential [11]. Seven ratios have been computed and are shown in Fig. 4. It should be stressed that the exponentially screened potential always has only a finite number of bound states increasing with the screening length ZD . Therefore high-angular excitations only exist for ZD sufficiently large. From Fig. 4 we find that all ratios are in agreement with our inequality (as they should). However, for large ℓ and large ZD , we find that some ratios lie slightly above the Coulomb ratios (this is invisible on the Figure). Since the error never exceeds 1 % the values are still within the claimed range of accuracy. As one could expect, the ratios are far away from the Coulomb case for small screening lengths ZD and come closer and closer to the Coulomb values as ZD increases.

Acknowledgements: One of us (J.S.) acknowledges the support of the Swiss National Science Foundation.

REFERENCES

1. M. Baumgartner, H. Grosse and A. Martin, *Phys.Lett.* **146B** (1984), 363.
2. M.S. Ashbaugh and R.D. Benguria, *Phys.Lett.* **131A** (1988), 273.
3. A. Martin, *Phys.Lett.* **147A** (1990), 1.
4. A.K. Common, *J.Phys.A:Math.Gen* **20** (1987), 4247.
5. A.K. Common and A. Martin, *Europhys.Lett.* **4** (1987), 1349.
6. A.K. Common and A. Martin, *J.Math.Phys.* **30** (1989), 601.
7. G.H. Hardy, J.E. Littlewood and G. Pólya, "Inequalities", 2nd edition, Cambridge 1957, Cambridge University Press.

8. J. Lee-Franzini, Private communication.
9. R. Engfer, H. Schneuwly, J.L. Vuilleumier, H.K. Walter and A. Zehnder, *Atomic Data and Nuclear Data Tables* **14** (1974), 509.
10. E. Borie and G.A. Rinker, *Rev.Mod.Phys.* **54** (1982), 67.
11. F.J. Rogers, H.C. Graboske, Jr. and D.J. Harwood, *Phys.Rev.* **A1** (1970), 1577.

FIGURE CAPTIONS

- 1) The ratios of transition energies between pure angular excitations of muonic atoms as a function of the nuclear charge Z .
- 2) Same as Fig. 1, but where particular combinations of transition energies corresponding to different spin states have been used to eliminate relativistic (Dirac) effects.
- 3) The level diagram of lithium, including the $4f \rightarrow 3d$ and $3d \rightarrow 2p$ transitions used in the text. Notice also the ordering of levels corresponding to a fixed principal quantum number, in connection with the BGM theorem.
- 4) Ratios of level spacings for an electron submitted to a screened potential as a function of $\delta = \frac{ZD}{a_0}$, where a_0 is the Bohr radius of hydrogen and D the screening length.

- Fig. 1 -

- Fig. 2 -

- Fig. 4 -

- Fig. 3 -