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**A NEW PROOF OF THE LOG-CONCAVITY PROPERTY OF
THE WAVE FUNCTION FOR A POTENTIAL
WITH LAPLACIAN OF A GIVEN SIGN**

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ABSTRACT

A new proof (the third!) of the fact that $\log(\frac{u}{r^{\ell+1}})$ is concave (convex), where u is the reduced ground state wave function, for angular momentum ℓ , solution of a Schrödinger equation with a potential such that its Laplacian is everywhere positive (negative) is given. This property is a crucial step in the proof that if the Laplacian is positive (negative) the levels belonging to a given Coulomb multiplet have energies decreasing (increasing) when the angular momentum increases.

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In 1984 [1] it has been shown that the energy levels associated to a Schrödinger equation with a central potential having an everywhere positive (negative) Laplacian are such that, for given $N = n + \ell + 1$, n number of nodes, ℓ angular momentum, the levels with higher ℓ have lower (higher) energy, i.e.,

$$E(n, \ell) \geq E(n-1, \ell+1) \text{ if } \Delta V \geq 0 \quad (1)$$

The proof makes use of a raising operator

$$A_{\ell}^{+} = \frac{d}{dr} - \frac{u'_{0,\ell}(r)}{u_{0,\ell}(r)} \quad (2)$$

where $u_{0,\ell}$ is the reduced ground state wave function of the Schrödinger equation with potential V and angular momentum ℓ . Then

$$A_{\ell}^{+} u_{n,\ell}(r) \quad (3)$$

where $u_{n,\ell}$ is the reduced wave function with n nodes, angular momentum ℓ , satisfies a Schrödinger equation with a potential $V + \delta V$, with the same energy, $n-1$ nodes, and angular momentum $\ell+1$. δV is given by

$$\delta V = - \left(\frac{u'}{u} \right)' - \frac{\ell+1}{r^2} \quad (4)$$

In (1) it has been shown that

$$\delta V \geq 0 \text{ everywhere if } \Delta V \equiv \frac{1}{r^2} \frac{dV}{dr} \geq 0 \quad (5)$$

Then, by using the property of monotonicity of the energy levels as functionals of the potential, it is easy to prove (1).

The proof of (5) given in Ref. [1] is not straightforward. It is made of several steps, distinguishing several cases, and though each step is elementary, the whole thing is unpleasant and many people have tried to find an alternative proof. Ashbaugh and Benguria [2] have succeeded to give an essentially algebraic proof after having made the observation that property (5) is equivalent to saying that $\eta = \log(\frac{r}{r_0})$ is concave (convex) when the Laplacian of the potential is positive (negative). They study a non-linear differential equation for η .

Here we shall push further the same idea and work directly with $\delta V = -v''$. Using the Schrödinger equation

$$-u'' + \left(\frac{\ell(\ell+1)}{r^2} + V - E \right) u = 0$$

we have

$$u^2 \delta V = (E - V)u^2 + u'^2 - \frac{(\ell+1)^2}{r^2} u^2 \quad (6)$$

and

$$\frac{d}{dr} [u^2 \delta V] = -\frac{dV}{dr} u^2 - 2uu' \frac{(\ell+1)}{r^2} + \frac{2(\ell+1)^2}{r^3} u^2$$

or

$$\frac{r^2}{u^2} \frac{d}{dr} [u^2 \delta V] = -r^2 \frac{dV}{dr} + 2(\ell+1) \left[-\frac{u'}{u} + \frac{\ell+1}{r} \right]$$

and hence, differentiating again

$$\frac{d}{dr} \left[\frac{r^2}{u^2} \frac{d}{dr} (u^2 \delta V) \right] = -\frac{d}{dr} r^2 \frac{dV}{dr} + 2(\ell+1) \delta V \quad (7)$$

In (7) we recognize $-\Delta V$ and, if $\Delta V \geq 0$ we have a linear differential inequality for δV :

$$\frac{d}{dr} \left[\frac{r^2}{u^2} \frac{d}{dr} (u^2 \delta V) \right] < 2(\ell+1) \delta V \quad (8)$$

Notice that $\lim_{r \rightarrow 0} u^2 \delta V = 0$, at least if the potential is such that $\lim_{r \rightarrow 0} r^2 V = 0$, because then $u \sim r^{\ell+1}$, and also $\lim_{r \rightarrow \infty} u^2 \delta V = 0$. To prove the latter one may use the fact that if the Laplacian has a given sign the potential is necessarily monotonous beyond a certain value of r . Then one can show that $u^2 \delta V$ has necessarily a limit and this limit can only be zero.

REFERENCES

1. B. Baumgartner, H. Grosse and A. Martin, *Phys.Lett.* **146B** (1984), 363.
2. M.S. Ashbaugh and R.D. Benguria, *Phys.Lett.* **131A** (1988), 273.

Assume now that there is an interval $r_1 < r < r_2$ where $u^2 \delta V < 0$ and such that $u^2 \delta V = 0$ at r_1 and r_2 . r_1 and r_2 could be 0 and ∞ . Then, by Rolle's theorem there exists r'_1, r'_2 :

$$r_1 \leq r'_1 < r'_2 \leq r_2$$

such that

$$\frac{r^2}{u^2} \frac{d}{dr} (u^2 \delta V)_{r'_1} < 0 \quad \frac{r^2}{u^2} \frac{d}{dr} (u^2 \delta V)_{r'_2} > 0$$

and again, by Rolle's theorem there is r'' ,

$$r_1 \leq r'_1 < r'' < r'_2 \leq r_2$$

such that

$$\frac{d}{dr} \left(\frac{r^2}{u^2} \frac{d}{dr} (u^2 \delta V) \right) > 0$$

which contradicts inequality (8). Since r_1 and r_2 can be taken to be 0 and/or ∞ , this covers all the cases where δV is somewhere negative on $0 \leq r \leq \infty$. Q.E.D.

For the case where $\Delta V \leq 0$ everywhere, the proof is identical.

However, in Ref. [1] we also proved the stronger result:

$$\delta V < 0 \quad \text{if} \quad \begin{cases} \text{either} & \frac{d}{dr} r^2 \frac{dV}{dr} \leq 0 \\ \text{and/or} & \frac{dV}{dr} \leq 0 \end{cases} \quad (9)$$

Then, if $\frac{dV}{dr} \big|_{r_0} < 0$ $\frac{dV}{dr}$ remains negative for $r > r_0$. Equation (5) can be written as

$$u^2 \delta V = \int_r^\infty u^2 \left\{ \frac{dV}{dr'} - \frac{2\ell(\ell+1)}{r'^3} \right\} dr' - \frac{\ell+1}{r^2} u^2$$

So if $r \geq r_0$, $u^2 \delta V$ is clearly negative. Then, if $u^2 \delta V$ is somewhere positive in $0 < r < r_0$, it vanishes at $r = r_1$ (which can be zero) and $r = r_2 < r_0$, and the previous argument works.