CERN-TH/95-152
LPTHE Orsay 95/32
ENSLAPP-A558-95
Revised Version

GENERALIZATION OF THE CALOGERO-COHN BOUND ON THE NUMBER OF BOUND STATES

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Abstract

It is shown that for the Calogero-Cohn type upper bounds on the number of bound states of a negative spherically symmetric potential $V(r)$, in each angular momentum state, that is, bounds containing only the integral $\int_0^\infty |V(r)|^{1/2}dr$, the condition $V'(r) \geq 0$ is not necessary, and can be replaced by the less stringent condition $(d/dr)[r^{1-2p}(-V)^{1-p}] \leq 0$, $1/2 \leq p < 1$, which allows oscillations in the potential. The constants in the bounds are accordingly modified, depend on p and ℓ, and tend to the standard value for $p = 1/2$.

CERN-TH/95-152
LPTHE Orsay 95/32
ENSLAPP-A558-95
October 1995

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I - Introduction

Among the numerous bounds on the number of bound states in a potential, or more generally the moments of the eigenvalues, physicists prefer those given by semi-classical expressions. Often these are only valid in the strong coupling limit and the price to pay to convert them into strict bounds is to multiply them by some appropriate numerical factor. In the case of the bound of Calogero and Cohn, who assume monotonicity of the potential, it is a factor two. What we shall show in this paper is that the requirement of monotonicity of the potential can be considerably weakened if one is ready to replace this factor two by a correspondingly larger one. This will broaden the field of application of the bound.

For a regular and spherically symmetric potential $V(r)$, which is purely attractive and nondecreasing ($V' \geq 0$), and vanishes at infinity, Calogero[1] and Cohn[2] have shown that in the S-wave, the number of bound states for the radial Schrödinger equation

$$\varphi'' + E\varphi = V\varphi \quad , \quad r \in [0, \infty) \quad , \quad \varphi(0) = 0 \tag{1}$$

admits the upper bound

$$n_0 \leq \frac{2}{\pi} \int_0^\infty |V(r)|^{1/2} dr \quad . \tag{2}$$

By regular potentials, we mean those which are less singular than r^{-2} at the origin, and go to zero faster than r^{-2} at infinity. More precisely, they satisfy the condition[3,4]

$$\int_O^\infty r|V(r)|dr < \infty \quad . \tag{3}$$

In what follows, we always assume that this condition is satisfied.

Recently, the bound has been generalized to higher angular momenta by taking into account the effect of the centrifugal potential $\ell(\ell+1)/r^2$, $\ell \geq 0$. One finds then, again, with the same conditions on the potential, namely (3) and $V' \geq 0$, the upper bound[5]

$$n_\ell \leq 1 + \frac{2}{\pi} \left[\int_0^\infty |V|^{1/2} dr - \sqrt{\left(\frac{\pi}{2}\right)^2 + \ell(\ell+1)} \right] \tag{4}$$

which reduces to (2) for $\ell = 0$.

For negative values of ℓ, $-1/2 < \ell \leq 0$, and again with the previous conditions on V, one has now[5]

$$n_\ell \leq \frac{1}{\sqrt{2(2\ell+1)}} \int_0^\infty |V|^{1/2} dr \quad . \tag{5}$$

Making $\ell = 0$ here, we do not get the Calogero-Cohn constant $2/\pi$, but $\sqrt{2}/2$, which is slightly larger. The above bound is singular for $\ell = -1/2$, and we shall see that this cannot be avoided.

With no condition on the potential, except (3), we have the general Bargmann bound[3,6]

$$n_\ell \leq \frac{1}{(2\ell+1)} \int_0^\infty r|V(r)|dr \tag{6}$$

This bound also has been generalized, again with no condition on potential except (3), to a large family of bounds[7]

$$n_\ell \leq \frac{C_p}{(2\ell+1)^{2p-1}} \int_0^\infty |r^2 V|^p \frac{dr}{r} \tag{7}$$

where p is a free parameter, $1 \leq p \leq 3/2$, and

$$C_p = \frac{(p-1)^{p-1}\Gamma(2p)}{p^p \Gamma^2(p)} \quad . \tag{8}$$

Making $p \downarrow 1$, we get the Bargmann bound (6), as expected. In (6) and (7), we have tacitly assumed V to be negative everywhere. If the potential changes sign, then we should replace in (6) and (7) V by its negative part V_-.

Now, the question arises whether one could fill the gap between (7), valid for $1 \leq p \leq 3/2$, and (2), (4), and (5), where we have the integral of $|V(r)|^p$, with $p = 1/2$. In short, whether one could find, with some condition on the potential - similar to the Calogero-Cohn condition $V' \geq 0$ - such that one would have a bound similar to (7) for $1/2 \leq p \leq 1$. The answer is in the affirmative. Indeed, assuming again V to be negative everywhere, and

$$\frac{d}{dr}\left[r^{1-2p}(-V)^{1-p}\right) \leq 0 \quad , \quad \frac{1}{2} \leq p \leq 1 \quad , \tag{9}$$

one can show that[8]

$$n_\ell \leq \frac{p}{(1-p)^{1-p}(2\ell+1)^{2p-1}} \int_0^\infty \left(-r^2 V\right)^p \frac{dr}{r} \quad . \tag{10}$$

We should remark here that again, for $p = 1$, (9) imposes no condition on the potential, and (10) gives us then the Bargmann bound (6), as expected. On the other hand, for $p = 1/2$, we obtain the Calogero-Cohn condition $V' \geq 0$, but then (10) goes to (5) with $\ell = 0$, which is slightly larger than (2), as we have noticed before.

For p strictly inside the interval $(1/2, 1)$, the potential may have oscillations while staying everywhere negative. As examples, we give just the two following ones[9] :

$$V_1 = -r^{(2p-1)/(1-p)} \; e^{-r/(1-p)} \quad ; \tag{11}$$

$$V_2 = -r^{(2p-1)/(1-p)} \left\{ \left[1 + \frac{1}{2}(\sin r + \cos r) \right] e^{-r} \right\}^{1/(1-p)} \quad . \tag{12}$$

It is easily seen that V_1, which vanishes at the origin, has a minimum before going to zero at $r = \infty$, whereas V_2 oscillates indefinitely while going to zero at $r = \infty$. Both satisfy (9).

The purpose of the present paper is to show that, in fact, condition (9) leads to a Calogero-Cohn type bound, for all $p \in [1/2, 1)$, that is, a bound containing the integral $\int_0^\infty \sqrt{|V|}dr$, but, of course, with a different constant than $2/\pi$. This would be much more satsifactory for strong attractive potentials since we know that, in the limit $\lambda \to \infty$, the number of bound states of λV, for any fixed $\ell \geq 0$, has the asymptotic behaviour[10,11]

$$n_\ell = \frac{\lambda^{1/2}}{\pi} \int_0^\infty |V_-|^{1/2} dr + \text{smaller terms} \quad , \tag{13}$$

with no condition on V than the finiteness of the integral.

II - General proof of a Calogero-Cohn type bound

Since we assume in general (3) and (9), we must have $\lim r^2 V(r) = 0$ as $r \to 0$ or $r \to \infty$. Now, (9) can be written

$$\frac{d}{dr} \left\{ \left[r^2(-V) \right]^{1-p} / r \right\} = -q(r) \tag{14}$$

where q is some positive function, and the function inside the bracket in the l.h.s. vanishes at infinity. Assuming $q(r)$ to be integrable there, which is quite natural, and solving the differential equation (14) for V, together with $V(\infty) = 0$, we obtain

$$V(r) = -r^{\frac{2p-1}{1-p}} \left(\int_r^\infty q(t)dt \right)^{\frac{1}{1-p}} \quad . \tag{15}$$

The only condition to be imposed on $q(r)$, besides being positive and integrable for $r > 0$, is that (3) must be satisfied. As examples, we can take $q(t) = e^{-t}$ or $q(t) = (1 + \sin t)e^{-t}$, and we obtain, respectively, (11) and (12).

We have now to deal with the radial Schrödinger at zero energy

$$\varphi_\ell'' = \left[V(r) + \frac{\ell(\ell+1)}{r^2} \right] \varphi_\ell \tag{16}$$

together with $\varphi_\ell(0) = 0$, and the well-known nodal theorem[3], which asserts that the number of bound states $n_\ell(V)$ is equal to the number of nodes (zeros) of $\varphi_\ell(r)$ on the real r-axis, origin excepted. The potential being given by (15), we can now use the Liouville transformation

$$r \to Z = r^{1/2(1-p)} \quad , \quad \varphi \to \psi(Z) = Z^{(2p-1)/2} \varphi(r(Z)) \quad . \tag{17}$$

The change of variable is one-to-one, and applies $r \in [0, \infty)$ on $Z \in [0, \infty)$, $r = 0$ corresponding to $Z = 0$. The change of function is such that to $\varphi(r = 0) = 0$ corresponds $\psi(Z = 0) = 0$. After the transformation, (16) becomes ($^{\cdot} = d/dZ$)

$$\ddot{\psi}(Z) = \left[\widetilde{V}(Z) + \frac{L(L+1)}{Z^2} \right] \psi(Z) \tag{18}$$

together with $\psi(0) = 0$, where

$$\widetilde{V}(Z) = -4(1-p)^2 \left(\int_r^\infty q(t) dt \right)^{\frac{1}{1-p}} \Bigg|_{r = Z^{2(1-p)}} \quad , \tag{19}$$

and

$$L = L(\ell, p) = -\frac{1}{2} + (1-p)(2\ell + 1) \quad . \tag{20}$$

We see that we have again to deal with a Schrödinger equation at zero energy, in the variable Z, with Dirichlet condition at the origin, and a potential $\widetilde{V}(Z)$ which is now attractive and increasing, together with the centrifugal term $L(L+1)/Z^2$. Moreover, the zeros of ψ on the positive Z-axis are in one-to-one correspondence with those of $\varphi(r)$ on the positive r-axis. It follows that the number of bound states is the same for (16) as for (18). However, the advantage of (18) is that we can now use the bounds (4) or (5), according to the value of $L \geq 0$, or $-\frac{1}{2} < L \leq 0$. We would then get bounds which contain $\int_0^\infty |\widetilde{V}(Z)|^{1/2} dZ$. This, expressed in terms of the variable r, is exactly $\int_0^\infty |V(r)|^{1/2} dr$, and we obtain the desired result. In résumé, we have the following

Theorem 1

Under the condition (9) on the potential, we have

$$n_\ell \leq 1 + \frac{2}{\pi} \left[\int_0^\infty |V(r)|^{1/2} dr - \sqrt{\left(\frac{\pi}{2}\right)^2 + L(L+1)} \right] \tag{21}$$

if L, given by (20), is ≥ 0, and

$$n_\ell \leq \frac{1}{\sqrt{2(2L+1)}} \int_0^\infty |V(r)|^{1/2} dr \tag{22}$$

if $L \in (-\frac{1}{2}, 0]$. The first case corresponds to $\ell \geq (2p-1)/4(1-p)$, and the second to $-1/2 < \ell \leq (2p-1)/4(1-p)$. We should remark here that when $\ell = 0$, we have $L = \frac{1}{2} - p$, which is negative, except for $p = \frac{1}{2}$, and so, we must use in general (22). If $\ell = 0$, and $p = \frac{1}{2}$, i.e. the Calogero-Cohn case, we have the bound (2), and don't have to use (22).

III - Direct proof of the generalized bound (22)

We consider the S-wave, described by equation (1). Suppose that there are n_0 bound states. This means that $\varphi_0(r)$ has n_0 nodes $0 < r_1 < \cdots r_{n_0} < \infty$. We assume now the potential to satisfy the following conditions :

$$V(r) \leq 0 \quad , \quad \left[-r^{-\nu}V(r)\right]' \leq 0 \quad \text{for some } \nu \geq 0 \quad . \tag{23}$$

We have now :

Lemma 1

If V satisfies (23), the same is true for $-V(r)(r-r_k)^{-\nu}$ for $r > r_k$. Indeed, we have

$$|V(r)|\,(r-r_k)^{-\nu} = \left[|V(r)|r^{-\nu}\right]\left(\frac{r}{r-r_k}\right)^{\nu} \quad ,$$

and both factors are decreasing for $r \geq r_k$. □

Now, from the Bargmann bound (6) with $\ell = 0$, we have

$$1 \leq \int_{r_k}^{r_{k+1}} (r-r_k)\,|V(r)|dr \quad .$$

Taking $\rho_k = r - r_k$, this can be written

$$1 \leq \int_0^{r_{k+1}-r_k} \rho_k W(\rho_k) d\rho_k \tag{24}$$

where $W(\rho_k) = V(\rho_k + r_k)$. Restricting ourselves to the interval (r_k, r_{k+1}), and dropping the index k, let us define

$$I(\rho) = \int_0^{\rho} \sqrt{|W(\rho')|}d\rho' \quad . \tag{25}$$

If V satisfies (23), Lemma 1 shows that $|W(\rho)|\rho^{-\nu}$ is also decreasing. Therefore

$$I(\rho) = \int_0^{\rho} \sqrt{|W(\rho')|\rho'^{-\nu}}\rho'^{\nu/2}d\rho' \geq \sqrt{\rho^{-\nu}|W(\rho)|} \times \frac{\rho^{1+\frac{\nu}{2}}}{1+\frac{\nu}{2}} = \rho\frac{\sqrt{|W(\rho)|}}{1+\frac{\nu}{2}} \quad . \tag{26}$$

Using now this inequality, together with (24) and $\frac{dI}{d\rho} = \sqrt{|W(\rho)|}$, we obtain

$$1 \leq \int_0^{r_{k+1}-r_k} \left[\rho\sqrt{|W(\rho)|}\right]\sqrt{|W(\rho)|}d\rho \leq \left(1+\frac{\nu}{2}\right)\int_0^{r_{k+1}-r_k} I(\rho)\frac{dI}{d\rho}d\rho =$$

$$\frac{1}{2}\left(1+\frac{\nu}{2}\right)\left[I\left(r_{k+1}-r_k\right)\right]^2 \quad .$$

Therefore

$$1 \leq \frac{\sqrt{\nu+2}}{2} I\left(r_{k+1}-r_k\right) = \frac{\sqrt{\nu+2}}{2} \int_{r_k}^{r_{k+1}} \sqrt{|V(r)|} dr \quad . \tag{27}$$

Adding up these inequalities for all the intervals, we end up with

$$n_0 \leq \frac{\sqrt{\nu+2}}{2} \int_0^\infty |V|^{1/2} dr \quad . \tag{28}$$

In order to apply this inequality to our potential satisfying (9), we just have to put $\nu = (2p-1)/(1-p)$. When p varies between $\frac{1}{2}$ and 1, ν varies between 0 and ∞. In any case, we obtain finally

$$n_0 \leq \frac{1}{2\sqrt{1-p}} \int_0^\infty |V(r)|^{1/2} dr \tag{29}$$

which is the desired result. □

Let us remark here that, for $p = 1$, the r.h.s. of (29) is infinite. Indeed, condition (9) for $p = 1$ puts no restriction on the potential. And with no restriction on the potential, the only bound which is valid in general is the Bargmann bound (6), which contains the integral of $|V|$ instead of $|V|^{1/2}$. As is well-known[3,6], the Bargmann bound can be saturated by n_0 negative δ-potentials with suitable strengths and locations :

$$V(r) = -\sum_{k=1}^{n_0} g_k \delta\left(r - r_k\right) \tag{30}$$

and such a potential gives zero in the r.h.s. of (29). It follows that the singularity at $p = 1$ in front of the integral in (29) cannot be avoided. We can summarize the results in the following

Theorem 2

For a purely attractive potential satisfying the condition (23) for some $\nu \geq 0$, the number of S-wave bound states satisfies the bound

$$n_0 \leq \frac{\sqrt{\nu+2}}{2} \int_0^\infty |V|^{1/2} dr \quad . \tag{31}$$

IV - Improvement of the Generalized Bound (22)

If $L = L(\ell, p) \in (-1/2, 0)$ we have the following operator inequality due to the local uncertainty principle[12]

$$-\frac{d^2}{dz^2} + \frac{L(L+1)}{z^2} \geq -(2L+1)^2 \frac{d^2}{dz^2} \ . \tag{32}$$

Hence the number of bound states of the operator associated to (18) is bounded above by the number of bound states of $(-2L+1)^2\frac{d^2}{dz^2}+\tilde{V}(z)$. Applying the Calogero-Cohn bound to this operator we find

$$n_\ell \leq \frac{1}{2L+1}\frac{2}{\pi}\int_0^\infty |V(z)||^{1/2}dr \ . \tag{33}$$

Together with (22) we therefore have

Theorem 3

Under the condition (9) on the potential and if $L\in(-1/2,0]$, we have

$$n_\ell \leq C_L\int_0^\infty |V(r)|^{1/2}dr \tag{34}$$

where

$$C_L=\min\left(\frac{1}{2L+1}\frac{2}{\pi},\frac{1}{\sqrt{2(2L+1)}}\right) \ . \tag{35}$$

If the potential satisfies condition (23) for some $V\leq 0$, the number of S-wave bound states satisfies the bound

$$n_0 \leq C_\nu\int_0^\infty |V(r)|^{1/2}dr \tag{36}$$

with

$$C_\nu=\min\left(\frac{\nu+2}{\pi},\frac{\sqrt{\nu+2}}{2}\right) \tag{37}$$

In particular

$$C_\nu=\left(\begin{array}{ll}\frac{\nu+2}{\pi} & \text{if} \quad \nu<\nu_C:=\frac{\pi^2-8}{4}\\ \frac{\sqrt{\nu+2}}{2} & \text{if} \quad \nu_C\leq\nu<\infty\end{array}\right) \tag{38}$$

We note that $\lim_{\nu\to 0}C_\nu=2/\pi$ so that we recover in the limit $\nu\to 0$ the optimal bound.

V - The case $0>\nu>-2$

From (31), we see that if the r.h.s. is less than 1, then there is no bound state. It is easy to see that this holds not only for $\nu>0$, but also for $0>\nu>-2$. In other words, if the absolute value of the potential decreases faster than $r^{-|\nu|}$, $0>\nu>-2$, then the condition

$$\frac{\sqrt{\nu+2}}{2}\int_0^\infty |V(r)|^{1/2}dr<1 \tag{39}$$

guarantees the absence of bound states. As an example, we can consider the Yukawa potential $V=-g\exp(-\mu r)/r$. Here, $\nu=-1$, and the constant in front of the integral becomes $1/2$, which is smaller than the Calogero constant $2/\pi$. However, we must remember that all this is derived from the Bargmann bound, and therefore we cannot do better than that. Also, generalization to n bound states for $\nu < 0$ is impossible because Lemma 1 no longer holds. So the interest of $\nu < 0$ is rather limited.

VI - The Calogero's sufficient condition

Here, we would like to see how good is the constant C_ν in front of (36). For this purpose, we consider the simple power-potential

$$V(r) = -\lambda r^\nu \theta(1-r) \quad . \tag{40}$$

Now, a sufficient condition of Calogero[13] states that, for a purely attractive potential, if there exists an R such that

$$\frac{1}{R}\int_0^R r^2|V(r)|dr + R\int_R^\infty |V(r)|dr \geq 1 \quad , \tag{41}$$

then there is at least one bound state. R is arbitrary here, and can be chosen at will. Applying (41) to (40), and maximizing with respect to R, we find that it is sufficient to have

$$\lambda \geq \lambda_1 = (\nu+2)\left[\frac{2(\nu+2)}{\nu+3}\right]^{\frac{1}{\nu+1}} \quad . \tag{42}$$

Now, assume that the r.h.s. of (36) is too large, and that C_ν can be replaced by a better (smaller) constant $\tilde{C}_\nu$. Applying now (36), with $n_0 = 1$ and the better constant $\tilde{C}_\nu$ to our potential (40), we find that we must have $\tilde{C}_\nu\sqrt{\lambda_1}\int_0^1 r^{\nu/2}dr \geq 1$, that is

$$\tilde{C}_\nu \geq \frac{(\nu+2)}{2\sqrt{\lambda_1}} > \left(\frac{\sqrt{\nu+2}}{2}\right)\left[\frac{\nu+3}{2(\nu+2)}\right]^{\frac{1}{2(\nu+1)}} \quad . \tag{43}$$

It is easily seen (see Appendix) that the factor $[(\nu+3)/2(\nu+2)]^{\frac{1}{2(\nu+1)}}$ is an increasing function of ν and goes to 1 as $\nu \to \infty$.

On the other hand the function $\frac{\pi}{2}\frac{1}{\sqrt{\nu+2}}\left[\left(\frac{\nu+3}{2(\nu+2)}\right]^{\frac{1}{2(\nu+2)}}$ is a decreasing function of ν (see Appendix). Therefore this example shows that our constant C_ν is not too bad, and that it cannot be improved more than by a factor $[(\nu_C+3)/2(\nu_C+2)]^{\frac{1}{2(\nu_C+1)}} = \left[\frac{1}{2}+\frac{2}{\pi^2}\right]^{\frac{2}{\pi^2-4}} \simeq 0.887$.

We should note here that the Schrödinger equation with the potential (40) can be solved exactly at zero energy. The regular solution is $\varphi = \sqrt{r}J_{L+\frac{1}{2}}(\sqrt{\lambda}Z)$, where $Z = r^{1+\frac{\nu}{2}}/\left(1+\frac{\nu}{2}\right)$, and $L = -\nu/2(2+\nu)$. The exact value of λ for which the first bound state appears is given by $\varphi'(r=1) = 0$. This is a transcendental equation whose solution is not simple, and needs numerical computation. In principle, this exact value of λ could be used instead of λ_1 of the Calogero's sufficient condition.

Acknowledgement

Two of us (K. C. and A. M.) would like to thank Masud Chaichian for warm hospitality at the Theoretical Physics Institute of the University of Helsinki where this work began.

Appendix

We must show that the derivative of $F(\nu) = [(\nu+3)/(\nu+2)]^{1/2(\nu+1)}$ is positive, which amounts to the same thing for the derivative of $G(\nu) = \log F(\nu)$. Now, if we write $H(\nu) = 2(\nu+1)^2 G'(\nu)$, we have

$$H(\nu) = \frac{1}{\nu+2} - \frac{2}{\nu+3} - \log\frac{\nu+3}{2(\nu+2)} \tag{A.1}$$

and, therefore,

$$H'(\nu) = (\nu+1)\left[\frac{1}{(\nu+2)^2} - \frac{1}{(\nu+3)^2}\right] > 0 \quad . \tag{A.2}$$

It follows that $H(\nu)$ is increasing for $\nu \geq 0$. Now,

$$H(0) \equiv 2G'(0) = \log\left(\frac{4}{3}\right) - \frac{1}{6} > 0 \quad . \tag{A.3}$$

Therefore, $H(\nu)$ is positive for $\nu \geq 0$, and the same is true for $G'(\nu)$. $\square$

Similarly, we consider the derivative of $\tilde{G}(\nu) = -\frac{1}{2}\log(\nu+2) + G(\nu)$. If we write $\tilde{H}(\nu) = 2(\nu+1)^2\tilde{G}'(\nu)$ we find

$$\tilde{H}(\nu) = -\frac{(\nu+1)^2}{\nu+2} + H(\nu) \tag{A.4}$$

and, therefore

$$\begin{aligned} \tilde{H}'(\nu) &= -\tfrac{(\nu+1)(\nu+3)}{(\nu+2)^2} + H'(\nu) \\ &= (\nu+1)\left[-\tfrac{1}{\nu+2} - \tfrac{1}{(\nu+3)^2}\right] < 0 \end{aligned} \tag{A.5}$$

Since $\tilde{H}(0) = \log\frac{4}{3} - \frac{2}{3} < 0$ it follows that $\tilde{H}(\nu) < 0$ for all $\nu \geq 0$.

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