

Bounds on the Number of Eigenvalues of the Schrödinger Operator

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Abstract. Inequalities on eigenvalues of the Schrödinger operator are re-examined in the case of spherically symmetric potentials. In particular, we obtain:

- i) A connection between the moments of order $(n - 1)/2$ of the eigenvalues of a one-dimensional problem and the total number of bound states N_n , in n space dimensions;
- ii) optimal bounds on the total number of bound states below a given energy in one dimension;
- iii) a lower bound on N_2 ;
- iv) a self-contained proof of the inequality

$$N_n < C_{\alpha n} \int \frac{dr}{r} (r^2 |V|_-)^{\alpha + n/2}$$

for $\alpha \geq 0, n \geq 3$, leading to the optimal $C_{04}, C_{\frac{1}{2}3}$;

v) solutions of non-linear variation equations which lead, for $n \geq 7$, to counter examples to the conjecture that C_{0n} is given either by the one-bound state case or by the classic limit; at the same time a conjecture on the nodal structure of the wave functions is disproved.

1. Introduction

There has been recently a great interest in bounds on the moments of the energy levels of the form [1]

$$\sum_{j=1}^N |e_j|^\gamma \leq M_{\gamma,n} \int dx x^{n-1} |V(x)|_-^{\gamma + \frac{n}{2}}. \tag{1}$$

Here e_j denotes the eigenvalues of $H = -\Delta + V(x)$ defined on $L^2(\mathbb{R}^n)$, $\hbar = 2m = 1$, and $|V|_-$ means the attractive part of V : $|V|_- = -V$ if $V < 0$ and zero otherwise. Notice that in our notation $M_{\gamma,n}$ is related to $L_{\gamma,n}$ of [1] by $M_{\gamma,n} = (2\pi^{n/2}/\Gamma(n/2))L_{\gamma,n}$, the proportionality factor being the surface of the n

dimensional sphere. As an application of such a bound let us note the proof of the stability of matter [2]. In [1], Lieb and Thirring proved Equation (1) for $\gamma > \max(0, 1 - n/2)$ and obtained the best possible constants in one dimension $M_{\gamma,1} = M_{\gamma,1}^c$ for $\gamma = \frac{3}{2}, \frac{5}{2}, \dots, 1$ where $M_{\gamma,1}^c$ denotes the ‘‘classical value’’ for $M_{\gamma,1}$ defined by

$$\left(\sum_j |e_j|^\gamma\right)_{\text{classical}} = \int \frac{d^n x d^n p}{(2\pi)^n} |p^2 + V|^\gamma = M_{\gamma,n}^c \int dx x^{n-1} |V(x)|^{\gamma + \frac{n}{2}} \tag{2}$$

so that $M_{\gamma,n}^c$ is given by (we denote $Cl_n = M_{0,n}^c$)

$$M_{\gamma,n}^c = \frac{\Gamma(\gamma + 1)}{\Gamma\left(\gamma + 1 + \frac{n}{2}\right) \cdot 2^{n-1} \cdot \Gamma\left(\frac{n}{2}\right)}. \tag{3}$$

Furthermore they conjectured that there exists a unique critical value of $\gamma (= \gamma_{c,n})$ such that

$$M_{\gamma,n} = M_{\gamma,n}^c \text{ for } \gamma \geq \gamma_{c,n}, \quad M_{\gamma,n} = M_{\gamma,n}^1 \text{ for } \gamma \leq \gamma_{c,n}, \tag{4}$$

where $M_{\gamma,n}^1$ denotes the optimal constant in (1) for $N = 1$. It has been proved that $\gamma_{c,1} = \frac{3}{2}$; it was conjectured (by numerical experiments) that $\gamma_{c,2} = 1.165$ and $\gamma_{c,3} = 0.8627$.

The problem of finding the best possible $M_{\gamma,n}$ remains open, and deserves some interest. For instance, if a bound similar to (4) holds for $\gamma = 1, n = 3$, for non-spherical symmetric V 's the bounds obtained in [2] on the ground state energy of matter can be seriously improved. In fact, as we shall see, conjecture (4) has to be modified, at least in spaces with dimension larger than 6.

For $\gamma = 0$ bounds like Equation (1) have been obtained by different methods [3]: first, partial results were given by Simon [4] and Martin [5]; Rosenblum's method [6] gives no constants, Cwikel's [7] is the most general one, and Lieb's approach [8] (using functional integrals) gives the best constants.

Here it will be shown that (for radial symmetric potentials) there exists a connection between $M_{0,n}$ and $M_{(n-1/2),1}$ in a sense to be made more precise below; in this way we add a proof of a finite bound on the number of bound states N_n . Furthermore bounds in one dimension imply a family of bounds in n dimensions; in this way we generalize our previously derived bounds of [9], where we obtained

$$M_{0,n}^1 = \frac{2 \cdot \Gamma(n)}{\Gamma\left(\frac{n}{2}\right) \cdot [n(n-2)]^{\frac{n}{2}}} \equiv S_n. \tag{5}$$

A procedure similar to that used in [9] gives us best possible bounds on the number of bound states below some non-zero energy in one dimension. As an amazing by-product we obtain a lower bound on N_2 .

In one dimension one can count the number of bound states using the nodal theorem. For n dimensions it is known that the wave function of the m^{th} energy state divides space at most into m disjoint nodal regions [10]. There are explicit examples, with potentials possessing some symmetry, where the number of nodal

¹ See however ‘‘Note Added in Proof’’

regions is less than m . However, a natural conjecture would be that small perturbations (small in some norm) lead always to a potential having the property that the m^{th} state divides space indeed into m regions; so one expects the last case to be the generic one. This would imply that the Sobolev constant (corresponding to $N = 1$) gives the best possible bound. However, we give examples of potentials violating the “nodal theorem” in $n \geq 7$ dimensions. These examples also disagree with the semi-classical result. So it turns out that the conjecture (4) is violated for $\gamma = 0$ and $n \geq 7$.

Conjecture (4) is also violated for $\gamma > 0$, sufficiently close to zero, $n \geq 7$. On the other hand, it may be completely correct in spaces with less dimensions and in particular for $n = 3$, where we have carried some numerical tests at $\gamma = 0.8627$ and seen near saturation, within 1% of (4) but no violation. On the basis of a partly heuristic variational argument, we propose a new conjecture for the case $\gamma = 0$.

2. Bounds on N_n and the One-dimensional Moment Problem

A) The first step involves a special counting of the number of negative energy states for the Schrödinger operator in n dimensions

$$[-\Delta + V(r)]\psi = e\psi. \tag{6}$$

After introducing the reduced wave function [11]

$$\psi(x) = r^{\frac{1-n}{2}} \chi(r) Y_l(x/r)$$

(6) reduces to

$$\left[-\frac{d^2}{dr^2} + \frac{\left(l + \frac{n-1}{2}\right)\left(l + \frac{n-3}{2}\right)}{r^2} + V(r) \right] \chi = e\chi, \tag{7}$$

where the degeneracy of each level is determined by the number of harmonic polynomials Y_l of degree l in n dimensions [11]:

$$D_l = H_l - H_{l-2}, \quad H_l = \binom{n+l-1}{l}. \tag{8}$$

Here H_l is the number of homogeneous polynomials of degree l in n dimensions.

We want to exploit the node theorem for radial wave functions: the number of bound states in a given angular momentum l will be equal to the number v_l of nodes of the zero energy solution of (7) multiplied by the degeneracy factor (8). If we look at the zero energy solutions regular at the origin as a function of the continuous parameter l (following Regge), we obtain a series of values of l (not necessarily integers)

$$l_{v_0} > l_{v_0-1} > \dots > l_1 \geq 0$$

for which the solution is also regular at infinity, and the corresponding number of nodes is $0, 1, \dots, v_0 - 1$. We evidently have

$$v_l = \sum_{i=1}^{v_0} \theta(l_i - l), \tag{9}$$

where $\theta(x) = 1, x \geq 0, \theta(x) = 0$ otherwise, and

$$N_n = \sum_{l=0}^{\infty} D_l v_l = \sum_i \sum_{l=0}^{[l_i]} D_l = \sum_{i=1}^{v_0} P([l_i], n) \tag{10}$$

$$P(l, n) = H_{l-1} + H_l = \frac{(n-2+l)!(n-1+2l)}{(n-1)!l!}.$$

B) We want now to transform the problem into a pure one-dimensional problem. Since we are interested only in zero energy solutions of (7) we can indeed make the substitution

$$z = \ln r \in (-\infty, \infty), \quad \phi = \frac{\chi}{\sqrt{r}}, \quad (r^2 V)(z) = v(z) \tag{11}$$

and look for the eigenvalues of the equation

$$\left[-\frac{d^2}{dz^2} + v(z) \right] \phi(z) = e_i \phi(z), \tag{12}$$

$$e_i = -\left(l_i + \frac{n-2}{2} \right)^2. \tag{13}$$

Now we may bound (10) by

$$N_n \leq K_{\sigma,n} \sum_i |e_i|^\sigma, \quad K_{\sigma,n} = \sup_l \frac{(n-2+[l])!(n-1+2[l])}{(n-1)!([l])! \left(1 + \frac{n-2}{2} \right)^{2\sigma}}, \tag{14}$$

where we are allowed to include e_i 's between zero and $-(n-2/2)^2$, which preserves the inequality. To get finite constants $K_{\sigma,n}$ we have to have $2\sigma \geq n-1$. If we now bound the moment of the sum of the energy levels in (14) by the appropriate norm of v with the right dimension (see Section 3)

$$\sum_i |e_i|^\sigma \leq M_{\sigma,1} \cdot \int_{-\infty}^{\infty} dz \cdot |v(z)|_{-}^{\sigma + \frac{1}{2}} \tag{15}$$

we obtain finally a family of bounds on $N_n \left(\sigma + \frac{1}{2} = \frac{n}{2} + \alpha \right)$

$$N_n \leq C_{\alpha,n} \int_0^{\infty} \frac{dr}{r} |r^2 V|_{-}^{\frac{n}{2} + \alpha}, \quad \forall \alpha \geq 0, \quad C_{\alpha,n} = K_{\sigma,n} \cdot M_{\sigma,1} < \infty. \tag{16}$$

C) To be able to exploit (15) and get bounds on N_n we need bounds on one-dimensional moments. In some cases optimal bounds are known as we mentioned it already in the Introduction, for $\gamma = \frac{3}{2}$, etc. Otherwise one could use the technique presented in [2] starting from the Birman-Schwinger [12] trace method to get a bound on $N_1(-\alpha)$, where $N_n(-\alpha)$ designates the number of bound states in n dimensions with energy less than $-\alpha$. In fact we can, by a straightforward extension of the methods of [9], derive a family of optimal upper bounds for $N_1(-\alpha)$.

For the sake of completeness we shall discuss this question in the general framework of [9]. In particular, in what follows, we do not need to assume spherical symmetry. In the course of our derivation some new bounds will appear, not explicitly contained in [9] and [1].

Let $V \in \mathcal{D}(R^n)$ and $\alpha \geq 0$ be given and let $\{\psi_j, e_j\}_1^N$ be the ordered set of bound states and corresponding energies of the Schrödinger operator $-\Delta + V$. Suppose j is fixed so that $e_j + \alpha \leq 0$. We write the corresponding Schrödinger equation in the form

$$-\Delta \psi_j + \alpha \psi_j = -V \psi_j + (e_j + \alpha) \psi_j. \tag{17}$$

Let us call $\psi_j^{-1}(0)$ the “nodal set” of the j^{th} eigenfunction. It is a closed set (ψ_j is continuous!) that decomposes R^n into n_j disjoint open connected components $\Omega_{\kappa}, \kappa = 1, \dots, n_j$:

$$R^n = \bigcup_{\kappa=1}^{n_j} \bar{\Omega}_{\kappa}.$$

The Ω_{κ} are called “nodal regions”. It is well known [10] that for the ground state $\psi_1^{-1}(0) = \emptyset$, i.e., $n_1 = 1$. Because of the orthogonality of the ψ_j 's, we have $n_j \geq 2$ for $j > 1$. A famous theorem due to Courant [10] tells us that $n_j \leq j$ in more than one dimension and $n_j = j$ for $n = 1$.

After these preliminary remarks we multiply (17) with ψ_j and integrate over any Ω_{κ} . Since ψ_j vanishes on $\partial\Omega_{\kappa}$ the first term on the left may be integrated by parts. If we drop the last term on the right-hand side, we obtain, because of $e_j + \alpha \leq 0$ the series of inequalities

$$\begin{aligned} \int_{\Omega_{\kappa}} d^n x [(V \psi_j)^2 + \alpha \psi_j^2] &\leq - \int_{\Omega_{\kappa}} d^n x V \psi_j^2 \\ &\leq \int_{\Omega_{\kappa}} d^n x r^{\beta} |V|_{-} r^{-\beta} \psi_j^2 \leq \|r^{\beta} V_{-}\|_{p, \kappa} \|r^{-\beta} \psi_j^2\|_{q, \kappa}. \end{aligned} \tag{18}$$

In the last step we have used the Hölder inequality with any $p \geq 1, p^{-1} + q^{-1} = 1$. $\|\cdot\|_p$ denotes the usual L^p norm with respect to the Lebesgue measure over R^n , the index κ denotes the corresponding norm over Ω_{κ} , $r = |x|$ and β is an appropriately chosen real number. In order that the inequality be meaningful, $\|r^{-\beta} \psi^2\|_{q, \kappa}$ must be $< \infty$ at least for all $\psi \in \mathcal{D}$, which gives the first necessary condition on β :

$$\beta \cdot q < n. \tag{19}$$

We divide the inequality (18) by $\|r^{-\beta} \psi_j^2\|_{q, \kappa}$ and we denote what we obtain on the far left by $F(X_{\kappa} \psi_j)$, X_{κ} = the characteristic function of Ω_{κ} , where F is the functional

$$F(\psi) = \frac{\|(V \psi)^2\|_1 + \alpha \|\psi^2\|_1}{\|r^{-\beta} \psi^2\|_q}. \tag{20}$$

If we suppose that the infimum of this functional taken over all $\psi \in \mathcal{D}(R^n)$ is a strictly positive number $\mu(\alpha)$, then, as will be shown presently, this number is necessarily of the form $\mu(\alpha) = \alpha^{+\delta} \mu(1)$, $\delta \geq 0$, and (18) becomes, after summing over all κ ,

$$n_j \leq \frac{\mu^{-p}(1)}{\alpha^{\gamma}} \int_{R^n} d^n x |r^{\beta} V_{-}|^p, \quad \gamma \geq 0. \tag{21}$$

This is the inequality we wanted to derive.

It remains to be seen under what conditions $\mu > 0$. For this purpose we take a fixed $\psi \in \mathcal{D}$, and minimize the function $(0, \infty) \in \sigma \rightarrow F(\psi_\sigma)$, where $\psi_\sigma(x) = \psi(x/\sigma)$. This function is of the form $A\sigma^a + B\sigma^b$ and we obtain

$$\begin{aligned}
 F(\psi) &\geq \alpha^{1-\theta} S(\psi) \\
 S(\psi) &= \frac{\|(\nabla\psi)^2\|_1^\theta \|\psi^2\|_1^{1-\theta}}{\theta^\theta (1-\theta)^{1-\theta} \|r^{-\beta}\psi^2\|_q} \tag{22}
 \end{aligned}$$

provided

$$0 < \frac{1}{2} \left(\frac{n}{p} + \beta \right) = \theta \leq 1. \tag{23}$$

We see that indeed

$$\delta = 1 - \theta \geq 0 \quad \text{and} \quad \gamma = (1 - \theta)p \geq 0. \tag{24}$$

From Equation (17) we get also the equation

$$e_j = \left\{ \int_{\Omega_*} d^n x [(\nabla\psi_j)^2 + V\psi_j^2] \right\} \left\{ \int_{\Omega_*} d^n x \psi_j^2 \right\}^{-1}$$

and if we submit the right-hand side to manipulations similar to (18), we obtain the inequality

$$|e_j|^\gamma \leq \frac{\mu^{-p}(1)}{n_j} \int_{\mathbb{R}^n} d^n x |r^\beta V|_p^\gamma, \quad \gamma = (1 - \theta)p \geq 0 \tag{25}$$

(compare with [1]), where $\mu(1)$ is the infimum of the same ‘‘Sobolev functional’’ $S(\psi)$ defined by Equation (22).

If $n > 1$, the simple argument presented in [9] shows that the condition

$$\beta > 0 \tag{26}$$

is also necessary in order to have $\mu > 0$. If the inequalities (19), (23), and (26) are respected, one can show by a slight generalization of the proof in [9] that the infimum of the functional S is attained by a spherically symmetric decreasing positive function $\psi(r)$ satisfying the corresponding variational equation

$$-\Delta\psi + a\psi - br^{-\beta} \psi^{2q-1} = 0 \tag{27}$$

with a, b two positive constants if $\theta < 1$, and $a=0, b > 0$ in the case $\theta=1$. In the latter case, which was treated in [9] for $n=3$, Equation (27) can be solved analytically and the numbers μ explicitly computed. Incidentally, these numbers give a lower bound for the general case, as can be seen by applying to $S(\psi)$ the Hölder inequality

$$\|r^{-\beta}\psi^2\|_q \leq \|r^{-\beta/\theta}\psi^2\|_{q_1}^\theta \|\psi^2\|_1^{1-\theta}, \quad q_1^{-1} = 1 - (\theta p)^{-1}.$$

If we make the ‘‘natural’’ conjecture mentioned in the Introduction, namely that in a generic potential $n_j=j$, we may replace n_j in inequality (21) by $N_{-\alpha}(V)$ = total number of bound states with $e \leq -\alpha$. This is certainly always true if

the right-hand side is ≤ 2 , but it is certainly false in general in the case of $n \geq 7$ dimensions, as shown by counter examples in the last section of this paper. It is again always true in the one-dimensional case. For $n=1, \beta=0$ we encounter a functional (20) which was treated in [9], so that

$$N_1(-\alpha) \leq \frac{C_p}{(\alpha t)^{p-\frac{1}{2}}} \int_{-\infty}^{\infty} dx |V(x) + (1-t)\alpha|^p \tag{28}$$

$$C_p = \frac{(p-1)^{p-1} \cdot \Gamma(2p)}{2^{2p-1} \cdot p^p \cdot \Gamma^2(p)}, \quad 0 < t \leq 1, \quad p \geq 1$$

[starting from Equation (17) we have subdivided α into two parts and included the part $(1-t)\alpha, 0 < t \leq 1$, into the potential]. For $t=1$ this is nothing but the inequality

$$v_l(V) \leq \frac{C_p}{\left(l + \frac{n-2}{2}\right)^{2p-1}} \int_0^{\infty} \frac{dr}{r} |r^2 V(r)|^p \tag{29}$$

of [9] for the total number of bound states of angular momentum l in a central potential $V(r)$. Equation (28) is obtained from (29) by replacing $(l + (n-2)/2)^2$ by $\alpha, r^2 V(r)$ by $V(x)$ where $x = \ln r$. [Strictly speaking, (29) was derived only for $n=3$, but the generalization to $n \geq 3$ is trivial.]

Inequality (28) is always better than inequality (2.8) of [2] except in the limiting case $p=1$ where they coincide. For $p \rightarrow \infty$ the improvement is a factor $e/2$.

From (28) one gets by integration non-optimal inequalities on the moments of the eigenvalues in one dimension :

$$\sum_i |e_i|^\gamma < \min_{\frac{1}{2} < m < \frac{3}{2}} Z(\gamma, m) \int_{-\infty}^{\infty} dz |V(z)|^{\gamma+\frac{1}{2}}$$

$$Z(\gamma, m) = \frac{(m-1)^{m-1} \Gamma(2m) \gamma^{\gamma+1} \Gamma(\gamma + \frac{1}{2} - m)}{2^{2m-1} m^{m-1} \Gamma(m) \Gamma(\gamma + \frac{3}{2}) (m - \frac{1}{2})^{m-\frac{1}{2}} (\gamma + \frac{1}{2} - m)^{\gamma+\frac{1}{2}-m}} \tag{30}$$

Typical values obtained in this way are

$$M_{1,1} \leq 1.269 \quad \text{for } m = 1.049, \tag{31}$$

$$M_{\frac{3}{2},1} \leq 0.870 \quad \text{for } m = 1.128$$

while the exact answer is $M_{\frac{3}{2},1} = 3/16 = 0.1875$.

3. Discussion, Examples

A) Let us concentrate on the celebrated bound $\alpha=0, n=3$, or the total number of bound states in three dimensions. Straightforward application of the technique described in the previous section leads to the inequality

$$M_{0,3} \leq K_{1,3} \cdot M_{1,1} = 4 \cdot M_{1,1} \tag{32}$$

[the maximum in (14) is reached for $l=0$] or, equivalently,

$$C_{0,3} = 4 \cdot M_{1,1} \tag{33}$$

Inequality (32) agrees perfectly with the conjecture (4) in the sense that if $M_{1,1}$ is given by the one-bound state inequality, the upper bound on $M_{0,3}$ in (32) coincides with the one-bound state inequality in three dimensions $M_{0,3} = 16/(3\sqrt{3\pi}) \cong 0.980$. So inequality (32) is optimal in a certain way.

However, if we do not want to make any assumption we have to use the result of Subsection 2C to control $M_{1,1}$. A brutal application of (31) and (32) would lead to

$$M_{0,3} \leq 5.076 \cong 5.18 \cdot M_{0,3}^1. \tag{34}$$

However, a more sophisticated approach allows some improvement. We write the number of bound states as

$$\begin{aligned} N_3 &= \sum_i ([l_i] + 1)^2 = \sum_i ([l_i] + \frac{1}{2})^2 + \sum_i ([l_i] + \frac{3}{4}) \\ &= \sum_i ([l_i] + \frac{1}{2})^2 + \frac{3}{4}v_0 + \sum_1^{[l_{v_0}]} v_k, \end{aligned} \tag{35}$$

where v_k is the number of bound states with angular momentum k without the multiplicity factor. Replacing v_0 and v_k by the bounds of [9] [Eq. (39)] and using

$$(2k + 1)^2 v_k \leq M_{0,3}^1 \int_0^\infty dr r^2 |V|^\frac{3}{2} \tag{36}$$

we get

$$\begin{aligned} N_3 &< \left(1.295 - \frac{1}{4} + \frac{\pi^2}{8} \right) \cdot M_{0,3}^1 \int_0^\infty dr r^2 |V|^\frac{3}{2} \\ &= 2.279 \cdot M_{0,3}^1 \int_0^\infty dr r^2 |V|^\frac{3}{2}. \end{aligned} \tag{37}$$

This particular bound is not quite as good as the bound obtained by Lieb [8] in which the coefficient in (37) is replaced by 1.49. However, as we shall see the situation is not the same in higher dimensions.

B) Strangely enough the connection between one dimension and n dimensions, when combined with the first Faddeev-Zakharov [13] sum rule for one dimension, leads to a *lower bound* for the number of bound states in two dimensional potentials. The first two sum rules are given by

$$- \int_{-\infty}^\infty dz V(z) = 4 \sum_i |e_i|^\frac{1}{2} + \int_{-\infty}^\infty dk T(k), \tag{38}$$

$$\int_{-\infty}^\infty dz V(z)^2 = \frac{16}{3} \sum_i |e_i|^\frac{3}{2} - 4 \int_{-\infty}^\infty dk k^2 T(k), \tag{39}$$

$$T(k) = \frac{1}{\pi} \ln(1 - R^2), \tag{40}$$

where $R < 1$ denotes the reflection coefficient, and $T \leq 0$. From (38) we get a lower bound of the form

$$\sum_i |e_i|^\frac{1}{2} \geq -\frac{1}{4} \int dz V(z) \tag{41}$$

Table 1. Bounds on $\sup_V \left(N_n / \int_0^\infty dx x^{n-1} |V|^{n/2} \right)$

N	m_{opt}	Example/ S_n	Example/ Cl_n	l_{opt}	Bound/ S_n	Bound/ Cl_n
1	1	1		0	1	
3	1	1		0	2.28	
4	1	1		0	1	
6	1	1		0	1.12	
8	4		1.36	2		1.42
10	8		1.24	5		1.28
12	13		1.18	10		1.21
14	20		1.15	16		1.16
16	28		1.12	23		1.14
18	37		1.11	32		1.12
20	47		1.09	42		1.10

which we may combine with (14), taking the $\inf(l)$ instead of the $\sup(l)$. For $n=2$ we need not worry about the constraint $|e_l| \geq (n-2)^2/4$ and obtain

$$N_2 \geq -\frac{1}{4} \int_0^\infty dr r V(r) . \tag{42}$$

This confirms the known fact that in two dimensions a purely attractive potential has always bound states.

C) In higher *even* dimensions, i.e., $n=4, 6, \text{etc.}$, we can exploit the fact that to get N_n , we need the moments of order $\frac{3}{2}, \frac{5}{2}, \text{etc.}$ in one dimension. The second Faddeev sum rule (39) allows to get the best possible bound for the moment of order $\frac{3}{2}$ leading (by using [14]) to

$$N_4 \leq \frac{3}{16} \int_0^\infty dr r^3 |V|^2 . \tag{43}$$

This is the best possible result which is saturated by the one-bound state condition. It agrees with conjecture (4).

Lieb and Thirring [2] have been able to prove that the higher moments, of order $\frac{5}{2}, \frac{7}{2}, \text{etc.}$, in *one* dimension are bounded by the ‘‘classical’’ value. The bounds thus obtained are presented in Table 1 and compared to the one-particle bound S_n for $n \leq 6$ and the classical bound for $n \geq 8$, Cl_n . The bounds are always larger than S_n and Cl_n . Furthermore for $n \geq 7$ the maximum of the right-hand side of Equation (14) is reached for an l value which differs from zero. We shall see in the next section that indeed for $n > 6$ the upper bound on N_n is necessarily above the classical bound.

D) In three dimensions we can also get an optimal result on $C_{\frac{3}{2},3}$ using the sum rule (39)

$$N_3 \leq \sum_i (l_i + \frac{1}{2})^3 \cdot \sup_l \frac{([l] + 1)^2}{(l + \frac{1}{2})^3} \leq \frac{3}{2} \int_0^\infty dr r^2 |V|^2 . \tag{44}$$

This agrees with the one-bound state inequality obtained in [9].

4. The Variational Approach. Examples and Conjectures

To get the best possible $C_{\alpha,n}$ and in particular $C_{o,n} = M_{o,n}$, one can try a variational method. We can set the problem in the following terms. Given N_n we can look for the infimum of

$$\int_0^\infty dr r^{n-1} |V|_r^{\frac{n}{2}} \tag{45}$$

when the number of bound states in n dimensions is larger or equal to N_n . To reduce the problem to a problem of minimum and to be able to write Lagrange variation equations it is necessary to prove first the *existence* of an absolute minimum.

It is indeed possible to prove the existence of an absolute minimum of (45) for given N_n , using the methods developed in Appendix B of [9], provided one adds the following artificial boundary conditions: the domain of definition of the Hamiltonian is defined to be $\varepsilon < |x| < R$ and the wave functions vanish at $|x| = \varepsilon$ and $|x| = R$. The bound states are defined to be states with energy ≤ 0 . Eventually one can let $\varepsilon \rightarrow 0$ and $R \rightarrow \infty$.

We shall not give the details of the proofs because, as we shall see, we shall not be able to carry out this program completely and use it only as a guide.

For the sake of generality let us assume that the existence of a minimum is established also in the class of non-spherically symmetric potentials $V(x) = -|V(x)|$ for the region $\Omega = \{\varepsilon < |x| < R\}$ with Dirichlet boundary conditions—we believe this to be true also, although we have not tried to prove it explicitly. Let $\{\psi_j, e_j\}_1^N$ be the corresponding eigenfunctions with non-positive eigenvalues.

Our first remark is that at least one of the energies e_j must be equal to zero. For if all $e_j > 0$, we multiply V by λ and decreasing λ from unity we increase continuously the energies of all the levels by the Feynman-Hellman theorem, decreasing thereby the integral (45), which is contradictory to our assumption. Therefore,

$$-\Delta\psi_j - |V|\psi_j = 0 \quad \text{for } j \in J, \tag{46}$$

where J is a non-empty subset of $\{1, \dots, N\}$.

We look now at a neighbouring potential $V' = V + \varepsilon g$, where ε varies in a neighbourhood of zero and $g \in \mathcal{D}(\Omega)$ is fixed. The energy levels will vary according to the so-called Feynman-Hellman formula

$$\delta e_j = - \int d^n x \delta |V| \psi_j^2 / \int d^n x \psi_j^2, \quad \delta = \left. \frac{\partial}{\partial \varepsilon} \right|_{\varepsilon=0}. \tag{47}$$

For every choice of g such that $\delta e_j < 0$ for all $j \in J$, we must have $\delta \int |V|^{n/2} \geq 0$, for otherwise (45) would not be minimal. As in the theory of Lagrange multipliers we conclude that

$$\delta \int |V|^{n/2} = - \sum_{j \in J} K_j \delta e_j$$

identically for all $g \in \mathcal{D}(\Omega)$, where K_j are some non-negative constants. Comparing the integrands, we obtain

$$|V| = \left(\sum_{j \in J} c_j \psi_j^2 \right)^{q-1}, \quad q = \frac{n}{n-2} \tag{48}$$

with c_j some non-negative constants. Among these at least one is strictly positive, because the Dirichlet operator $-\Delta_\Omega$ has notoriously strictly positive eigenvalues for any bounded Ω , which would contradict our assumptions. By changing the normalization of the ψ_j 's and comparing with (46), we find that the minimizing V is of the form

$$V = -\lambda \left(\sum_{j=1}^M \psi_j^2 \right)^{q-1}, \quad q = \frac{n}{n-2}, \quad \lambda > 0, \tag{49}$$

where the $\{\psi_i\}_1^M$ satisfy the system of non-linear differential equations

$$-\Delta \psi_i - \lambda \left(\sum_{j=1}^M \psi_j^2 \right)^{q-1} \psi_i = 0, \quad i = 1, \dots, M \tag{50}$$

and the boundary condition $\psi_i|_{\partial\Omega} = 0$. Here it is understood that some of the ψ_i 's—but not all—may be identically zero. For the sake of convenience—see the Appendix—the constant λ was not normalized to 1.

We note that (50) are the variational equations corresponding to stationary points of the functional

$$F(\boldsymbol{\psi}) = \left\{ \int_\Omega \sum_1^M (V\psi_j)^2 d^n x \right\} \cdot \left\{ \int_\Omega \left(\sum_1^M \psi_k^2 \right)^q d^n x \right\}^{-\frac{1}{q}} \tag{51}$$

and that at these stationary points $F(\boldsymbol{\psi}) = \|V\|_p$, $p = n/2$, where V is defined by (49). Thus (51) and (50) are the natural generalization of the functional (20) and the corresponding variational Equation (27) for the one-bound state problem (for the case $\beta = 0$, $p = n/2$, $\alpha = 0$). It is also easy to see that the infimum of (51) is equal to that of (20) (all ψ_j equal to zero except one).

If we restrict ourselves to the class of spherically symmetric potentials, then any zero-energy solution is necessarily of the form

$$\psi_j = R_l(r) Y_{l,m}(x/r)$$

with at most one R_l in each angular momentum l , but with m running over all “magnetic quantum numbers” pertaining to this l . Also there is only a finite number of angular momenta for which we can have bound states in the minimizing potential due to the case $p = n/2$ of the inequality (29). If we normalize the spherical harmonics so that

$$\sum_m Y_{l,m}^2(x/r) = 1$$

and use the “logarithmic variables” (11), we get from (49) and (50) for the minimizing potential $v(z)=(r^2V)(z)$ the equation

$$v = -\lambda \left(\sum_{l=0}^L \phi_l^2 \right)^{q-1}, \quad q = n/n-2, \quad \lambda > 0, \tag{52}$$

where the functions $\{\phi_l\}_0^L$ satisfy the set of non-linear equations

$$-\phi_l'' + \left(l + \frac{n-2}{2} \right)^2 \phi_l - \lambda \left(\sum_{i=0}^L \phi_i^2 \right)^{q-1} \phi_l = 0, \quad l=0, \dots, L \tag{53}$$

and the boundary condition $\phi_l(z_1) = \phi_l(z_2) = 0, l=0, \dots, L$, where $z_1 = \ln \varepsilon, z_2 = \ln R$. Here it is again understood that some ϕ_l —but not all—may be identically equal to zero. It is also clear that these equations may be obtained directly within the framework of the restricted problem.

In what follows we shall discuss in some detail the spherically-symmetric case.

a) The Case of Only One Zero Energy State with Angular Momentum L at the Minimum

The system (53) reduces to the single differential equation

$$-\phi_L'' + \left(L + \frac{n-2}{2} \right)^2 \phi_L - (\phi_L)^{\frac{n+2}{n-2}} = 0. \tag{54}$$

The solutions of this equation are known and actually discussed for the special case $n=3$ in Appendix B of [9]. The point is that (54) admits a first integral:

$$-(\phi_L')^2 + \left(L + \frac{n-2}{2} \right)^2 \phi_L^2 - \frac{n-2}{n} (\phi_L)^{\frac{2n}{n-2}} = \text{const} \tag{55}$$

from which solutions can be constructed. In the case of $\varepsilon \rightarrow 0, R \rightarrow \infty$, i.e., of the infinite interval in z , there is only a one-parameter family of solutions vanishing for $|z| \rightarrow \infty$ such that the “potential” is

$$Vr^2 = v = - \frac{n \left(L + \frac{n-2}{2} \right)^2}{n-2} \left[\cosh \left(\frac{2L+n-2}{n-2} \right) \cdot (z-z_0) \right]^{-2}. \tag{56}$$

The parameter z_0 expresses the translation invariance of Equation (54). If, instead of taking an infinite interval one takes a finite interval, corresponding to $\varepsilon > 0, R < \infty$, Equation (56) admits a sequence of periodic solutions given by elliptic functions. A solution with $\nu_L - 1$ zeros between $\log \varepsilon$ and $\log R$ will correspond to ν_L bound states with angular momentum L counted without the multiplicity factor. For $\nu_L \ll \log(R/\varepsilon)$ this solution can be approximated by superpositions of solutions of the type (56) with

$$z_0 - \log \varepsilon \cong \frac{1}{2\nu_L} \log \frac{R}{\varepsilon}, \quad \frac{3}{2\nu_L} \log \frac{R}{\varepsilon} \text{ etc., } \dots$$

Since the case of v_L bound states with angular momentum L differs from $v_L = 1$ only by an over-all factor and by small corrections it is enough to treat the latter case.

To count the number of bound states for the potential of Equation (56), we may use Equation (10). The angular momenta l_i for which zero energy states appear can be obtained from the known eigenvalues of

$$\left[-\frac{d^2}{dz^2} - \frac{\beta^2 \lambda(\lambda-1)}{\text{ch}^2 z \beta} \right] \varphi = \varepsilon \varphi, \quad \varepsilon = -\beta^2 [\lambda - 1 - m]^2$$

$$m = 0, 1, 2, \dots, \tag{57}$$

where m has to be less or equal to $\lambda - 1$. Comparing (57) to (56) gives

$$\lambda = \frac{n}{2}, \quad \beta = \frac{2L}{n-2} + 1. \tag{58}$$

So it is easy but tedious to count all bound states and compare them to S_n for $n \leq 7$ and to Cl_n for $n \geq 8$. For $n = 3$ and 4 only one zero-energy state appears ($l_i = L$) and we obtain

$$\frac{N_3}{I_3} = \frac{(L+1)^2}{(2L+1)^2} S_3, \quad \frac{N_4}{I_4} = \frac{(2L+1) \cdot (L+2)}{2(L+1)^2} S_4, \tag{59}$$

where I_3 and I_4 are special cases of

$$I_n = \int_{-\infty}^{\infty} dz |v|^{\frac{n}{2}}. \tag{60}$$

The conclusion from (59) is that the optimum is obtained if all bound states have angular momentum zero, which corresponds to the fact that the sup in Equation (14) is obtained for $l = 0$. For $n = 5$ and 6 one arrives at the same conclusion but has to distinguish between two different cases and obtains eventually two contributions. For $n \geq 7$ on the other hand, one obtains already a violation of the conjecture (4) (for $\lambda = 0$) on which we will comment next.

b) The Case of m Zero-Energy States

Unfortunately there is no reason why zero-energy bound states of the minimizing potential should appear only in one angular momentum. In the general case we may have zero-energy states for a certain number of different angular momenta and we must investigate the system of differential Equations (53).

In principle we should find all solutions of (53) with boundary conditions $\phi_i(Z) = \phi_i(-Z) = 0$ and study the limit $Z \rightarrow \infty$. By different methods (explained in the Appendix) we found solutions to (53) with boundary conditions at infinity (which means zero energy). In all cases the potential turns out to be of the shape of (56). On the one hand we did not finish completely this program, on the other hand, with the help of these examples, we were able to check the conjecture (4) for $\gamma = 0$. For the solutions of (53) one can sum up the bound states as before and obtains:

$$\left(\frac{N_n}{I_n} \right)_m \frac{1}{Cl_n} = \frac{2^{n-1} (n+m-2)! (n+2m-2)}{[(n+2m-2)(n+2m-4)]^{\frac{n}{2}} (n-1)!}, \tag{61}$$

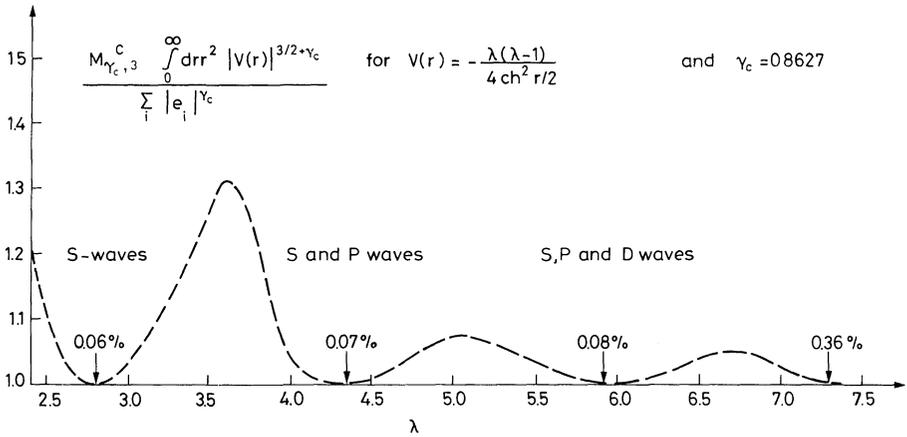


Fig. 1

where m denotes the number of equations in (53). The result of the optimization in m together with our bounds is given in Table 1. For $3 \leq n \leq 7$ we have to compare (61) to the Sobolev constants S_n . For $n \geq 7$ our examples violate the Sobolev bound which would result if the nodal theorem were true. We believe that the numbers obtained from (61) after optimization in m are the best possible. So the new conjecture is that up to $n=6$ the Sobolev constants will be the best possible. For higher n the best answer will be given by the optimizing m of (61) and for $n \rightarrow \infty$ the classical value will be reached.

To test the conjecture that $M_{\gamma_c, 3} = M_{\gamma_c, 3}^c$ we calculated the eigenvalues of the potential

$$V(r) = -\frac{c^2 \lambda(\lambda - 1)}{ch^2 cr} \tag{62}$$

and compared the γ_c moment with the appropriate norm of V . The conjectured inequality turns out to be nearly saturated for different coupling constants corresponding to the cases of different angular momentum contributions (see Fig. 1).

Appendix

Here we would like to show ways of getting solutions of systems of equations like (53). We may include the angular depending parts and even count states differing only by magnetic quantum numbers separately. In this way we arrive at the system

$$-\Delta \psi_i - \lambda \left(\sum_{j=1}^M |\psi_j|^2 \right)^{\frac{2}{n-2}} \psi_i = 0, \quad i = 1, \dots, M. \tag{A.1}$$

A stereographic projection to the n dimensional sphere imbedded into R^{n+1} :

$$\xi_0 = \frac{1-r^2}{1+r^2}, \quad \xi_i = \frac{2x_i}{1+r^2}, \quad i = 1, \dots, n, \quad r^2 = \sum_{i=1}^n x_i^2 \tag{A.2}$$

transforms the n dimensional Laplacian into the angular momentum operator on the sphere [14]:

$$-\left(\frac{1+r^2}{2}\right)^2 \Delta = \left(\frac{1+r^2}{2}\right)^{-\frac{n-2}{2}} \left(l^2 + \frac{n(n-2)}{4}\right) \left(\frac{1+r^2}{2}\right)^{\frac{n-2}{2}}, \tag{A.3}$$

$$l^2 = l_{\alpha\beta} l^{\alpha\beta}, \quad l_{\alpha\beta} = -i\xi_\alpha \frac{\partial}{\partial \xi_\beta} + i\xi_\beta \frac{\partial}{\partial \xi_\alpha}. \tag{A.4}$$

Defining new wave functions

$$\chi_i = \left(\frac{1+r^2}{2}\right)^{\frac{n-2}{2}} \psi_i. \tag{A.5}$$

(A.1) turns into the non-linear system of equations on the sphere

$$\left[l^2 + \frac{n(n-2)}{4} - \lambda \left(\sum_{j=1}^M |\chi_j(\xi)|^2 \right)^{\frac{2}{n-2}} \chi_i(\xi) = 0, \quad i = 1, \dots, M. \right] \tag{A.6}$$

Comparing (A.6) with the eigenvalue equation for l^2 in n dimensions

$$l^2 Y_{pm} = p(p+n-1) Y_{pm}, \quad p = 0, 1, \dots \tag{A.7}$$

and observing that the generalized spherical harmonics fulfil the completeness relation

$$\sum_m Y_{pm} Y_{pm}^* = 1 \tag{A.8}$$

(the sum runs over all magnetic quantum numbers), we find solutions for special values of the coupling constant λ :

$$\lambda = \frac{n+2M-2}{2} \cdot \frac{n+2M-4}{2}, \quad M = 1, 2, 3, \dots \tag{A.9}$$

We obtained the same solutions by a different method. This time we started directly with the system (53):

$$-\phi_i'' + \left(l_i + \frac{n-2}{2}\right)^2 \phi_i - \lambda \left(\sum_j \phi_j^2\right)^{\frac{2}{n-2}} \phi_i = 0. \tag{A.10}$$

For $i=1$ $l_1=0$ the solution to (A.10) is well known

$$\phi_{(n)} = \frac{c_{(n)}}{(\text{ch } z)^{\frac{n-2}{2}}}. \tag{A.11}$$

Assuming that solutions to the coupled systems are polynomials in $\phi_{(n)}$ and $d\phi_{(n)}/dz$ to the potential $\lambda\phi_{(n)}^{4/(n-2)}$ we may start with the ansatz

$$\phi_{i,(n)} = \sum_m c_{m,i} \phi_{(n)}^m \quad \text{or} \quad \phi_{i,(n)} = \sum_m d_{m,i} \phi_{(n)}^{m-1} \frac{d\phi_{(n)}}{dz}. \tag{A.12}$$

In both cases one gets recurrence relations for the coefficients; the overall constants for the wave functions are fixed by the subsidiary condition

$$\sum_i \phi_{i,(n)}^2 = \phi_{(n)}^2. \quad (\text{A.13})$$

By the uniqueness theorem for linear systems of differential equations it is evident that solutions obtained by the last procedure are identical to those obtained from (A.7).

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Note Added in Proof

Recently we have been informed that M. Aizenman and E. Lieb (unpublished) have proven

$$M_{\gamma,1} = M_{\gamma,1}^e \quad \text{for all } \gamma \geq 3/2.$$

With the help of this result one can improve our bounds for odd dimensions ($n \geq 5$).