Zeitschrift: Helvetica Physica Acta
Band: 45 (1972)
Heft: 2

Artikel: Bound states in the strong coupling limit
Autor: Martin, André
DOI: https://doi.org/10.5169/seals-114373

Helvetica Physica Acta
Vol. 45, 1972 Birkhäuser Verlag Basel

Bound States in the Strong Coupling Limit

by **André Martin**

CERN, Geneva

(23. XII. 71)

Abstract. We show that the number of bound states of a particle in a short-range potential in n dimensions is given asymptotically by

$$N = g^{n/2} \frac{S_n}{(2\pi)^n} \int \left| \frac{2MV^-}{\hbar^2} \right|^{n/2} d^n x + 0(g^{n/2-\varepsilon})$$

for $g \to \infty$, where gV^- is the attractive part of the potential, and S_n is the volume of the n dimensional sphere with unit radius.

1. Introduction

One of the fields which has been explored by the theoreticians in Zürich and in particular by Markus Fierz is that of Strong Coupling Theory. The strong coupling theory constitutes the first serious attempt to avoid the inconsistent application of perturbation theory to hadron physics. At the present time we are still looking for a good method to attack the problem of strong interactions. In the meantime we can play with the strong coupling situation in Schrödinger theory. It is amusing and it may even be useful.

The problem we want to discuss here is that of the number of bound states of a potential gV in n dimensions when g goes to infinity. After the classical work on the problem of bound states for finite g [1], the problem of $g \to \infty$ has been investigated and solved in *one dimension* by successive contributions of Calogero [2], Frank [3], Chadan [4] and Mourre [5]. One finds that the number of bound states behaves like

$$g^{1/2}/\pi \int \sqrt{|V^-(r)|}\,dr \tag{1}$$

where gV^- is the attractive part of the potential (we set $2M/\hbar^2 = 1$). Then Simon [6] was able to find bounds for spherically symmetric potentials in three dimensions by using the remark that for sufficiently large l the centrifugal termwill be everywhere larger than the potential if $\sup r^2|V^-(r)|$ exists. In this way Simon finds bounds behaving like $g^{3/2}$ for large g.[1])

[1]) B. Simon has also shown that $l_{\max}$, the maximum angular momentum for which one has a bound state in the case of three dimensions with spherical symmetry is such that, for a potential gV

$$\lim_{g\to\infty} \frac{l_{\max}^2}{g} = \sup|r^2\, V^-(r)|$$

Here we want to find the analogue for n dimensions of the asymptotic formula of Chadan for one dimension, without assuming spherical symmetry, for short range potentials, i.e., excluding the n body system which *has not a short range interaction* as seen in $3n$ dimensions because the interaction is not zero if two particles are close from one another even if a third particle is far away.

To make life simple we shall assume what is probably more than what we need, for instance, that the interaction has a strictly finite range, is bounded below and satisfies a Hölder continuity condition:

$$|V(x) - V(y)| < |x-y|^{\alpha} C \quad 0 < \alpha \leqslant 1. \tag{2}$$

In the last section we sketch the procedure to weaken these assumptions.

As we shall see the main tool we shall be using is the minimax principle of Weyl [7] which we shall discuss in the next section.

2. The Minimax Principle

In its standard form it is this. Let D_k be a k dimensional subspace in a space of square integrable functions rapidly decreasing at infinity which will be otherwise specified, and H a Hamiltonian. Then

$$\sup_{\psi \in D_k} \frac{(\psi H \psi)}{(\psi\psi)}$$

is larger than the kth eigenvalue of H, and the infimum over all possible D_k is indeed the kth eigenvalue.

Now to be able to make such a statement one has to know something about the Hamiltonian! In what follows we shall admit that the Hamiltonian is well behaved, i.e., that it has only bound states with negative energy, in finite number and with finite multiplicity. It is very likely that the assumptions we have made about the potential (lower bound and vanishing of the interaction beyond a certain distance) are sufficient to ensure this.[2]) Anyway, here, we shall admit these nice properties and proceed further.

Then, the minimax principle can be reduced to the ordinary variational principle: for $k = 1$ we are reduced to the problem of minimizing $(\psi H \psi)/(\psi|\psi)$ and this minimum is attained by the ground state ϕ_0.

For $k = 2$ D_k has two basic vectors ψ_1 and ψ_2 and we consider

$$\psi = \psi_1 (\phi_0|\psi_2) - \psi_2 (\phi_0|\psi_1)$$

which is orthogonal to the ground state, and gives a lower bound of $\sup (\psi H \psi)/(\psi|\psi)$ inside D_k. Minimizing with respect to ψ_1, ψ_2 will give the first excited state, etc.

Precautions have to be taken in case of degeneracy of the levels but since we have assumed that levels have a finite multiplicity this produces only a finite amount of complication.

---

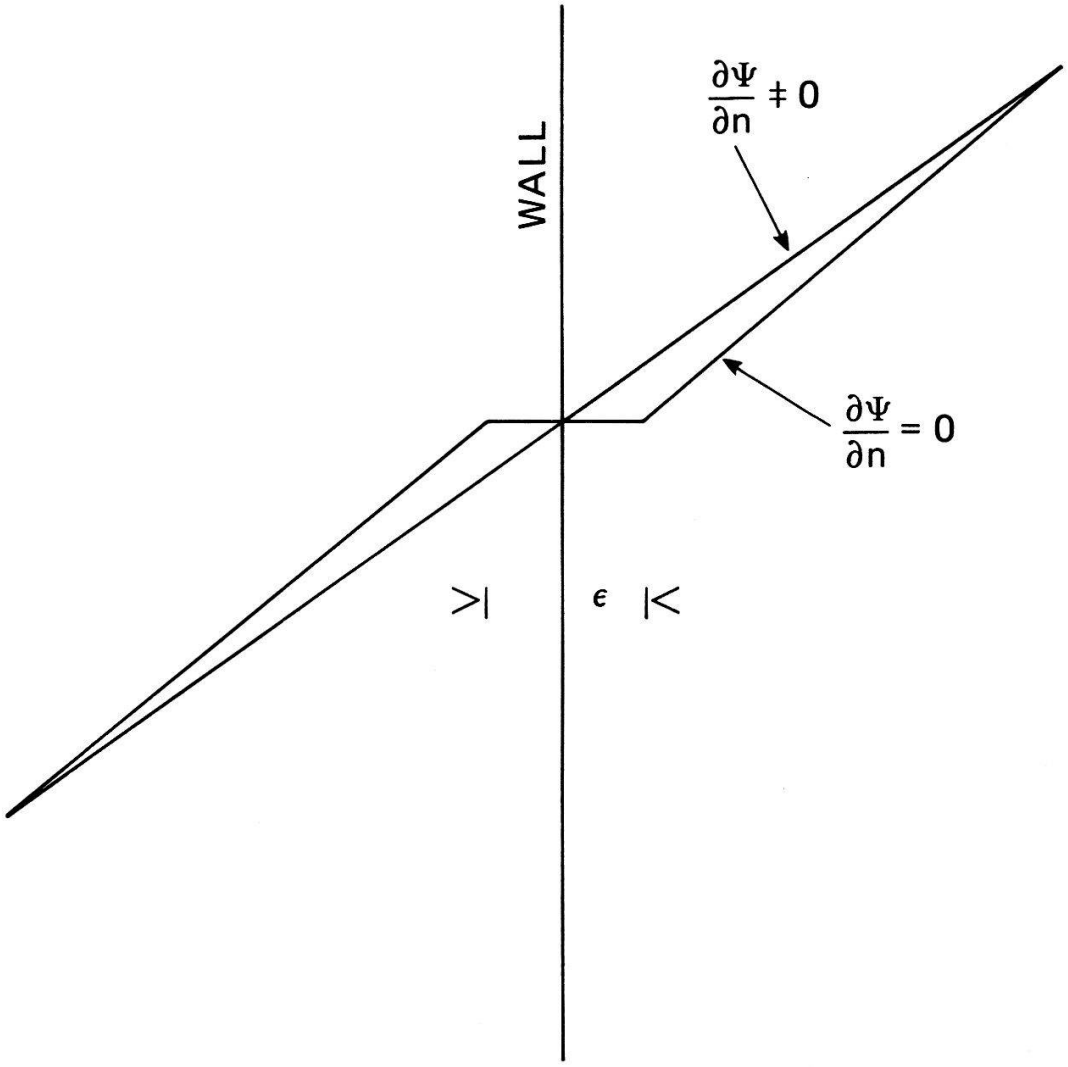
[2]) The discreteness and finite degeneracy of the levels for negative energy are guaranteed by an argument to be found in Courant-Hilbert, Vol. 1, pp. 448–450, generalized by W. Hunziker in Helvetica Phys. Acta *39*, 451 (1966). That zero energy is not an accumulation point can be proved by using our method: first one counts the number of levels up to an energy $-\epsilon$ and one shows that the upper bound, if $\epsilon \to 0$ stays finite.

Now we shall be more specific and write explicitly the Hamiltonian

$$H = -\Delta + V(x) \tag{3}$$

with

$$\hbar^2/2M = 1$$



where Δ is the n dimensional Laplacian. Then by partial integration for functions sufficiently differentiable and vanishing at infinity we can write

$$\frac{(\psi H \psi)}{(\psi|\psi)} = \frac{\int (|\nabla\psi|^2 + V(x)|\psi|^2)dx\,.}{\int |\psi|^2\,dx} \tag{4}$$

It is this expression which will be used in the minimax principle and *not* the original one. In this way we can work with the class of functions vanishing at infinity with bounded (but not necessarily continuous) first derivatives.

Now an important remark: if we restrict the class of functions to which we apply the minimax principle we restrict the possible D_k and, therefore, raise the minima corresponding to the various k's. For instance, demanding that ψ vanishes on a plane will modify the problem and lead to an algebraic increase of the energy levels. However, as

was pointed out to me once by D. Robinson, demanding that the ψ's one works with have a vanishing normal derivative along a plane *will not change* the levels obtained from the minimax principle, *if one uses the form* (4) (after partial integration). Indeed, one can approach as closely as one wishes a function with non-vanishing normal derivative by a function with vanishing normal derivative in such a way that $\int |\nabla\psi|^2 dx$ is changed as little as one wishes as illustrated on the figure. However, we must add a word of caution. The integration by parts leading to (4) is legitimate only because ψ vanishes at infinity and the integrated term goes away. If one works in a finite domain in x space it is legitimate if either ψ or $d\psi/dn$ vanishes on the *border* of the domain. Fortunately these are the only two kinds of boundary conditions that we shall use.

3. Lower Bound on the Number of Energy Levels

The idea is extremely simple: we divide the region where the potential is non-vanishing in cubic cells and impose on the trial ψ's that they vanish on the walls of the cells. This restricts the space in which we can take the D_k's in the minimax principle and, therefore, raises the levels. The number of bound states is, therefore, larger than the total number of levels of the individual wells up to zero energy. Further, we still reduce this number if in each individual well we replace $V(x)$ by $\sup V(x)$. Then we have reduced the problem to counting the levels of an n dimensional cubic well with infinite walls, i.e., to a known problem. The asymptotic formula for the number of levels up to momentum k in a cubic well of size d:

$$N(k) = S_n \left(\frac{dk}{2\pi}\right)^n - C_n (dk)^{n-1} + 0(dk)^{n-2} \tag{5}$$

In three dimensions it is [8], [9]

$$N(k) \cong \frac{(dk)^3}{6\pi^2} - \frac{3}{8}\frac{(dk)^2}{\pi} + 0(k)^3) \tag{6}$$

---

[3]) The formulae for the number of levels up to k^2 inside a cube of side

$$N(k) \cong \frac{(dk)^3}{6\pi^2} \mp \frac{3}{8}\frac{(dk)^2}{\pi} + \frac{3}{4\pi}(dk)$$

(depending on the boundary conditions) are smoothed expressions and do not represent lower or upper bounds. There are *jumps* in the correct $N(k)$ which are given by the maximum number of points with integer co-ordinates on a sphere of radius dk/π. These jumps have been estimated as follows. Let $r(n)$ be the number of ways of decomposing n into two squares (Hardy and Wright, The Theory of Numbers, 3rd Edition, p. 240). The number of points on a sphere of radius R is

$$r(R^2) + 2[r(R^2-1) + r(R^2-4) + \cdots + r(R^2-n^2) + \cdots]$$

Now it can be shown that $r(n) \leqslant 4d(n)$, number of divisors of n, and $d(ab) \leqslant d(a)\,d(b)$. Therefore

$$2\sum_0^R r(R^2-n^2) \leqslant 2\sum d(R-n)\,d(R+n) \leqslant \sum_0^R [(d(R-n))^2 + (d(R+n))^2] = \sum_{p=1}^{2R} |d(p)|^2$$

The latter quantity, according to Ramanujan (same reference, p. 265) is of the order of $R(\log R)^3$. The maximum amplitude of the fluctuations of $N(k)$, for both boundary conditions is therefore at most of the order of $(kd)\,(\log (kd))^3$.

Now we have to count the total number of states in the various cells. If $gV_i = \sup[gV(x)]$ in the ith cell is negative, this cell contains at least

$$N_i = S_n \left(\frac{d\sqrt{g|V_i|}}{2\pi} \right)^n - C_n (d\sqrt{g|V_i|})^{n-1}$$

bound states and, hence, we get

$$N > \frac{S_n}{(2\pi)^n} \sum_{i, V_i < 0} d^n (\sqrt{g|V_i|})^n - \frac{1}{d} \sum_{i, V < 0} d^n (\sqrt{g|V_i|})^{n-1}. \tag{7}$$

Now we must turn (7) into an integral. What we have to do is to use the Hölder condition (2), which tells us that inside a cell:

$$|V_i - V(x)| < Cd^\alpha$$

Then we get

$$N > \frac{S_n}{(2\pi)^n} g^{n/2} \int dx |V_-(x)|^{n/2} - \frac{C_n}{d} g^{n/2-1} \int dx |V_-(x)|^{n/2-1/2}$$
$$- D_n' d^\alpha g^{n/2} \int dx |V_-(x)|^{n/2-1} \tag{8}$$

Now we must adjust d as a function of g in such a way that for $g \to \infty$ the leading term becomes the first one. One finds, with $d = \text{const} g^{-1/(2(1+\alpha))}$

$$N > \frac{S_n}{(2\pi)^n} g^{n/2} \int dx |V_-(x)|^{n/2} - \text{const}\, g^{n/2 - \alpha/2(\alpha+1)}. \tag{9}$$

In the best possible case, $\alpha = 1$ and the corrective term is of the order of $g^{-1/4}$ with respect to the main one.

4. Upperbound on the Number of Bound States

Here we shall again use the division in cells but instead of putting walls where ψ vanishes we demand that the ψ's have a zero normal derivative on these walls. The first thing to do is to reduce the problem to a problem in a finite region. We enclose the interaction region in a cube, demanding that the trial ψ's have $\partial\psi/\partial n = 0$ on the faces of the cube. Then, if $\psi \in D_k$ we have

$$E_k = \inf_{D_k} \left\{ \sup_{\psi \in D_k} \frac{\int [|\nabla\psi_{\text{int}}|^2 + V(x)|\psi_{\text{int}}|^2] dx + \int |\nabla\psi_{\text{out}}|^2 dx}{\int |\psi_{\text{int}}|^2 dx + \int |\psi_{\text{out}}|^2 dx} \right\} \tag{10}$$

where E_k is the kth level of our problem, since the restriction $\partial\psi/\partial n = 0$ on the cube plays no role. $\nabla\psi_{\text{int}}$ and ψ_{int} coincide with $\nabla\psi$ and ψ inside the cube and are set equal to zero outside. ψ_{out} and $\nabla\psi_{\text{out}}$ have a similar meaning. Equation (10) shows that if

$$\sup_{\psi \in D_k} \frac{\int |\nabla\psi_{\text{int}}|^2 + V(x)|\psi_{\text{int}}|^2 dx}{\int |\psi_{\text{int}}|^2 dx}$$

is *negative* then we necessarily get an *underestimate* of E_k by suppressing the terms containing ψ_{out} and $\nabla\psi_{\text{out}}$. Therefore, we get

$$E_k \leqslant E_{k\,\text{int}} \quad \text{if} \quad E_{k\,\text{int}} < 0 \tag{11}$$

where

$$E_{k\,\text{int}} = \inf_{D_k}\left\{\sup_{\psi \in D_k} \frac{\int(|\nabla\psi_{\text{int}}|^2 + V|\psi_{\text{int}}|^2)dx}{\int|\psi_{\text{int}}|^2\,dx}\right\}.$$

The $E_{k\,\text{int}}$ are the energies of the problem limited to the cube with vanishing normal derivative. Therefore, the number of bound states is less or equal to the number of states with negative energy inside the cube. From now on we shall be able to work on the interior problem which has the advantage of having a purely discrete spectrum.

Now we proceed to divide the cube in cells. It is enough to see what happens when we split it in two parts, imposing $\partial\psi/\partial n = 0$ at the interface. This part of the argument is due to V. Glaser.

We drop the index 'int'. We call ψ_{L} a function which coincides with ψ in the left part, and ψ_{R} a function which coincides with ψ in the right part. The levels in the left are $E_{\text{L}_1} E_{\text{L}_2} \ldots$ etc., in the right $E_{\text{R}_1} E_{\text{R}_2} \ldots$ etc. Assume that if we consider the union (in increasing order) of the E_{L_i} and E_{R_i} we find among the first k levels pE_{L_i}'s and $k-pE_{\text{R}_i}$'s, with $E_{\text{L}_p} < E_{\text{R}_{k-p}}$. We have

$$\frac{(\psi H\psi)}{(\psi\psi)} = \frac{(\psi_{\text{L}} H\psi_{\text{L}})}{(\psi_{\text{L}}\psi_{\text{L}})} \times \frac{(\psi_{\text{L}}\psi_{\text{L}})}{(\psi_{\text{L}}\psi_{\text{L}}) + (\psi_{\text{R}}\psi_{\text{R}})} + \frac{(\psi_{\text{R}} H\psi_{\text{R}})}{(\psi_{\text{R}}\psi_{\text{R}})} \frac{(\psi_{\text{R}}\psi_{\text{R}})}{(\psi_{\text{L}}\psi_{\text{L}}) + (\psi_{\text{R}}\psi_{\text{R}})}$$

i.e., $(\psi H\psi)/(\psi|\psi)$ is a convex combination of $(\psi_{\text{L}} H\psi_{\text{L}})/(\psi_{\text{L}}|\psi_{\text{L}})$ and $(\psi_{\text{R}} H\psi_{\text{R}})/(\psi_{\text{R}}|\psi_{\text{R}})$.

Now we take ψ belonging to the space D_k

$$\psi = \lambda_1\psi_1 + \lambda_2\psi_2 + \cdots + \lambda_k\psi_k.$$

Then

$$\frac{(\psi_{\text{L}} H\psi_{\text{L}})}{(\psi_{\text{L}}\psi_{\text{L}})} = \frac{H_{\text{L}}(\lambda)}{D_{\text{L}}(\lambda)}$$

where $H_{\text{L}}(\lambda)$ and $D_{\text{L}}(\lambda)$ are quadratic forms, D_{L} being a positive quadratic form. Then we look for the eigenvalues of the quadratic form $H_{\text{L}}(\lambda)$ with respect to $D_{\text{L}}(\lambda)$,

$$\epsilon_{q\text{L}} = \inf_{E_q \subset C_k}\left\{\sup_{\lambda \in E_q} \frac{H_{\text{L}}(\lambda)}{D_{\text{L}}(\lambda)}\right\}.$$

E_q being a subspace of the λ's of dimension q. To each $\epsilon_{q\text{L}}$ is associated an eigenvector

$$e_{q\text{L}} = \sum \lambda_{iq\text{L}}\psi_i.$$

Here we forget about possible degeneracies. If we now choose ψ in the $k-p$ dimensional subspace

$$e_{p+1,\text{L}}\, e_{p+2,\text{L}} \cdots e_{k,\text{L}}$$

we have the certainty that $(\psi_L H\psi_L)/(\psi_L \psi_L)$ will be larger than $\epsilon_{p+1,L}$ but $\epsilon_{p+1,L}$ is itself larger than $E_{p+1,L}$ since we have been working on a particular k dimensional space. Hence, choosing ψ in the $k-p$ dimensional space $e_{p+1,L} \ldots e_{kL}$ guarantees

$$\frac{(\psi_L H\psi_L)}{(\psi_L \psi_L)} > E_{p+1,L}.$$

Once this is done we can maximize $(\psi_R H\psi_R)/(\psi_R|\psi_R)$ when ψ is in the space $e_{p+1,L} \ldots e_{kL}$. Then by the minimax principle

$$\frac{(\psi_R H\psi_R)}{(\psi_R \psi_R)} > E_{k-p,R}$$

ψ is now entirely fixed inside the space D_k and $\psi H\psi/\psi\psi$ being a convex combination of the right and left contributions we get

$$\sup_{\psi \in D_k} \left\{\frac{(\psi H\psi)}{(\psi\psi)}\right\} > \frac{(\psi H\psi)}{(\psi\psi)} > \inf \begin{cases} E_{p+1,L} \\ E_{k-p,R}. \end{cases}$$

Minimizing now with respect to the possible D_k's we get

$$E_k > E_{k\,\mathrm{int}} > \inf \begin{cases} E_{p+1,L} \\ E_{k-p,R} \end{cases}$$

i.e., $E_{k-p,R}$ with the present configuration, which means that there are in the union of the right and left wells k levels below the kth level of the complete problem.

We have skipped the problem of degeneracies. These degeneracies can be removed by arbitrarily small *negative* perturbations of V which necessarily *increase* the number of bound states.

One can continue the subdivision in cells. At each step the number of bound states increases.

Now we need to know the number of states in a cubic cell of side d with $\partial\psi/\partial n = 0$ on the sides. It is [8], [9]

$$N(k) \simeq S_n \left(\frac{dk}{2\pi}\right)^n + C_n (dk)^{n-1} + 0(dk)^{n-2} \quad [4]) \tag{12}$$

in particular in three dimensions it is

$$N(k) \lesssim \frac{(dk)^3}{6\pi^2} + \frac{3}{8\pi}(dk)^2 + \frac{3}{4\pi}(dk). \tag{13}$$

We can now repeat what we did in the last section calling V_i' the lower bound of $V(x)$ in the ith cell. We sum over all cells where V_i' is negative [it may be that in one cell $V(x)$ is partly positive, partly negative, but this cell must be included in the summation]. We get

$$N < \frac{S_n}{(2\pi)^n} \sum_i d^n |V_i'|^{n/2} + \frac{1}{d} C_n \sum_i d^n |V_i'|^{n/2-1/2}. \tag{14}$$

[4]) See previous footnote.

We turn this discrete sum into an integral with the help of the Hölder condition and of the inequality

$$||V(x)|^\nu - |V(y)|^\nu| \leqslant 2^{\nu-1}[|V(x) - V(y)||V(y)|^{\nu-1} + |V(x) - V(y)|^\nu]. \tag{15}$$

We get

$$\begin{aligned} N < \frac{S_n}{(2\pi)^n} g^{n/2} \int dx |V_-(x)|^{n/2} + C_n \frac{g^{n/2-1}}{d} \int dx |V_-(x)|^{n/2-1/2} \\ + D_n g^{n/2} d^\alpha \int dx |V_-(x)|^{n/2-1} + E_n g^{n/2} d^{\alpha n/2} \Omega \\ + F_n g^{n/2-1} d^{\alpha-1} \int dx |V_-(x)|^{n/2-3/2} + G_n g^{n/2-1} d^{\alpha n/2} \Omega \\ + H_n g^{n/2-1} d^{\alpha(n/2-1/2)-1} \Omega \end{aligned} \tag{16}$$

where Ω is the volume of the interaction region. Of this horrible expression only the first terms are really important for $n \geqslant 2$. As before we set

$$d = \text{const} \times g^{-1/2(\alpha+1)}$$

and get

$$N < \frac{S_n}{(2\pi)^n} g^{n/2} \int dx |V_-(x)|^{n/2} + 0(g^{n/2-\alpha/2(\alpha+1)}). \tag{17}$$

5. Conclusion and Remarks

Comparing (9) and (17) we get the asymptotic behaviour of the number of bound states

$$N \sim \frac{S_n}{(2\pi)^n} g^{n/2} \int dx |V_-(x)|^{n/2}. \tag{18}$$

In particular we get back the result of Chadan for $n = 1$. For $n = 3$ the factor $g^{3/2}$ agrees with the bounds of Simon, but we get of course a much more precise result. It is therefore tempting to test the accuracy of (18). The simplest *non-trivial* test is to compare (18) with the exact formula for a square spherical well. Then (18) reduces to

$$N \sim \frac{2}{9\pi}(kR)^3 \quad \text{where} \quad k = \sqrt{\frac{2MV}{\hbar^2}}.$$

For $kR = 7$ we get $N = 24{,}2$ while the exact result is 30 states (counted with their multiplicity!). For $kR = 18$ we get $N = 412{,}5$ instead of 424 states.

We would like to point out that (9) and (17) can be made completely accurate, i.e., strict bounds if one works with sufficient care, using strict bounds for the level density formulae in wells with infinite walls.

We would also like to express our belief that the asymptotic formula (18) has been derived under too strong conditions. One should be able to allow for isolated singularities provided they are not too strong and leave the integral convergent. One should also be able to allow potential extending to infinity provided it decreases fast enough. In the

latter case one has of course to prove first that all bound states of our problem have negative energies, but apart from this the problems of comparison with square wells are not terribly difficult. One must just vary the size of the cells, and take them small where the potential is large and large where the potential is small, in such a way to get always convergent series. Of course, then, something more flexible must replace the Hölder condition, something like

$$|V(x) - V(y)| < |x - y|^{\alpha}[C + |V(x)| + |V(y)|]. \tag{19}$$

Finally, we would like to mention a somewhat related problem whose solution is known [9]. If one takes a fixed potential which, instead of vanishing grows to infinity when $|x|$ goes to infinity, one can count the number of levels up to $E = \lambda$. This is

$$N_{\lambda} \sim \frac{S_n}{(2\pi)^n} \int dx |\lambda - V(x)|^{n/2} \tag{20}$$

integrated over the region where $\lambda - V$ is positive. This formula resembles very much (18). However, it must be understood that a quite different limit is being taken.

Estimates like (18) or (20) are not purely academic. For instance, in a recent work on systems of particles with Newtonian interactions W. Thirring and G. Hertel [10] have used a bound of the type (18). (20), on the other hand, is very useful when one wants to apply the Kato methods to interactions dominated by an anharmonic oscillator, in n dimensions, which means that it may become useful in constructive field theory.

6. Acknowledgments

I would like to thank K. Chadan, through whom I got interested in the problem, D. Robinson for an illuminating lecture on the minimax principle a few years ago, B. Simon and W. Hunziker for useful information and, finally, V. Glaser, for supplying the key of the proof of section 3. I thank Mr. Wim Klein for some numerical calculations.

REFERENCES

[1] V. Bargmann, Proc. nat. Acad. Sci. U.S.A. *38*, 961 (1952); F. Calogero, Nuovo Cim. *36*, 199 (1965); J. Schwinger, Proc. nat. Acad. Sci. U.S.A. *47*, 122 (1961).
[2] F. Calogero, Comm. Math. Phys. *1*, 80 (1965).
[3] W. M. Frank, J. Math. Phys. *8*, 466 (1967).
[4] K. Chadan, Nuovo Cim. *58A*, 191 (1968).
[5] K. Chadan and E. Mourre, Nouvo Cim. *64A*, 961 (1969).
[6] B. Simon, J. Math. Phys. *10*, 1123 (1969).
[7] H. Weyl, Nachr. Akad. Wiss. Göttingen *110* (1911); see also R. Courant and D. Hilbert, Meth. math. Phys. *1*, p. 132.
[8] R. Balian and C. Bloch, *Saclay Preprint*, to appear in Ann. Phys.
[9] C. Clark, SIAM Rev. *9*, 627 (1967).
[10] G. Hertel and W. Thirring, *CERN Preprints TH. 1330 and 1338*, to appear in Comm. Math. Phys.