Commun. math. Phys. 53, 221—231 (1977)

Communications in
Mathematical
Physics

Inequalities on the Number of Bound States in Oscillating Potentials

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Abstract. For short-range oscillating potentials $V(r)$, such that $W(r) = -\int_r^\infty V(r')dr'$ possesses some regularity properties we establish inequalities on the number of bound states. In particular we show that by replacing $V(r)$ by $-4(W(r))^2$ in the classical inequalities we get bounds for this new class of potentials. Optimal bounds are also obtained. The behaviour for large coupling constants is studied.

1. Introduction and Outline

The purpose of this paper is to obtain upper bounds for the number of bound states of a class of spherically symmetric potentials introduced recently by Baeteman and one of us (K.C.) [1]. These potentials, although very singular and oscillating near the origin, are perfectly regular from the point of view of quantum scattering theory. In fact, it was even shown that the usual description of scattering via the Jost function applies to this class as well, without any modification, and therefore that this class generalizes the notion of regular potential. A further generalization has been made to non-spherical potentials by Combescure and Ginibre [2].

In this paper, we are concerned with the spherically symmetric case, and assume always that the potential has a short range, i.e., it decreases faster than r^{-2} at large distances. More precisely, we assume that $V(r)$ is real, locally integrable away from the origin, and that

$$\int_a^\infty r|V(r)|dr < \infty , \qquad \forall a > 0 . \tag{1}$$

Traditionally, regular spherically symmetric potentials were those for which rV is absolutely integrable at the origin, i.e.,

$$\int_0^\infty r|V(r)|dr < \infty \tag{2}$$

[a possible, slightly different version is $\lim_{r\to 0} r^2|V(r)| = 0$].

Then it follows that $u_l(r)$, the regular solution of the reduced radial Schrödinger equation ($\psi_l = u_l(r)/r$) behaves like r^{l+1} at the origin, that the spaces of incoming and outgoing states are complete, and that therefore the scattering matrix is well-defined and is unitary [3]. Another case where all these nice properties hold is that of singular *repulsive* potentials, i.e., those which are more singular than r^{-2} at the origin. In this case, the regular and physically acceptable wave function vanishes faster than any power of r at the origin.

The new extension of the notion of regular potentials at the origin is as follows: instead of assuming (2), we assume only (1), but we require in addition that the absolutely continuous function

$$W(r) = -\int_r^\infty V(t)dt\,, \qquad r>0 \tag{3}$$

is such that

$$\lim_{r\to 0} rW(r) = 0 \tag{4}$$

and

$$W\in L^1(0,b)\,, \qquad b>0\,. \tag{5}$$

In short, if V is singular and oscillatory near the origin such that (2) is violated, we assume that the oscillations are controlled in an appropriate way as to satisfy (4) and (5). Notice that, because of (1), we also have

$$W\in L^1(0,\infty) \tag{6}$$

and

$$rW^2 = (rW)W\in L^1(0,\infty)\,. \tag{7}$$

Then the scattering matrix has all the nice properties one wants, and the scattering problem as well as the inverse scattering problem can be formulated exactly in the same way as for potentials satisfying (2). The reasons why potentials satisfying (1), (4), and (5) should also be called regular are the following:

i) if V has a constant sign near the origin, (1), (4), and (5) are equivalent to (2);

ii) in contradistinction with the case of truly repulsive singular potentials, the reduced radial wave function behaves like cr^{l+1}, $c\neq 0$, at the origin;

iii) if we multiply the potential by a "coupling constant" g, and make $g\to -g$, the character of the potential does not change in our case; in fact the S matrix is an analytic function of g around $g=0$; this is again in contradistinction with the case of truly singular repulsive potentials.

As an example, let us mention simply the following:

$$W(r) = r^{-1/2}\sin(e^{1/r})e^{-\mu r}\,. \tag{8}$$

Differentiating this expression to get the potential, one sees that it is highly singular and oscillatory at the origin, such that

$$\int_0 rV_\pm(r)dr = \infty\,, \tag{9}$$

where

$$V_{\pm}(r) = |V(r)|\theta(\pm V(r)) . \tag{10}$$

It is now clear that the classical bounds on the number of bound states for regular potentials satisfying (2) are not valid in the present case. For instance, the Bargmann bound on the number of bound states with angular momentum l [4]

$$v_l \leqq (2l+1)^{-1} \int_0^\infty rV_-(r)dr \tag{11}$$

no longer holds. One of us (K.C.) has already shown [4] that in the $l=0$ state the number of bound states for the present case satisfies the bound

$$v_0 \leqq 2 \int_0^\infty r(W(r))^2 dr . \tag{12}$$

This is of course valid for higher l, too, but does not decrease with increasing l, as it should do for obvious reasons.

In the present paper, we would like to make a more systematic study of the problem. First, we shall prove that in all standard bounds using the spherical symmetry of the potential, we can make the substitution

$$V(r) \to -4(W(r))^2 \tag{13}$$

and get a bound for the new family of potentials. Specifically, if $v_l(V)$ designates the number of bound states with angular momentum l in the potential V, we prove in Section 2:

$$v_l(V) < v_l(-4W^2) . \tag{14}$$

The inequality obtained in this way is not optimal. However, by using minimization methods analogous to those of Glaser et al. [5] we find in Section 3 least upper bounds for $v_l(V)$ in terms of W. Saturation of these bounds is explicitly established. However, one gets the same qualitative behaviour of v_l as a function of l as in Section 2. Finally, in Section 4 we discuss the coupling constant dependence of the bound and show that by using a slightly strengthened version of condition (4) one can establish that the number of bound states in the $l=0$ state grows at most like g for a potential gV.

2. The Substitution $V(r) \to -4\,(W(r))^2$

We shall take advantage of the fact that the potential is spherically symmetric in the usual way, namely by using the property that the number of bound states in angular momentum l is given by the number of nodes of the radial solution of the Schrödinger equation, regular at $r=0$, at zero energy. This fact is so well known that it is very difficult to trace back its first demonstration. It is therefore necessary to give a proof which holds for the new class of potentials we are considering, satisfying conditions (1) and (3)–(5). The explicit proof given by one of us (K.C.) and Montes [6], which uses the continuous motion of the zeros of the regular wave function when the momentum k varies, can be easily extended to this new situation. So we leave it as an exercise to the reader to make the necessary modifications in [6].

Consider the situation where we have ν_l bound states with angular momentum l. The reduced zero energy wave function satisfies

$$u'' - Vu - r^{-2}l(l+1)u = 0. \tag{15}$$

If we integrate (15) between two successive zeros of u, r_p, r_{p+1} we get

$$0 = \int_{r_p}^{r_{p+1}} (u'^2 + r^{-2}l(l+1)u^2 + Vu^2)dr. \tag{16}$$

On the other hand, we can integrate the last term in (16) by parts and get, using definition (3):

$$0 = \int_{r_p}^{r_{p+1}} [u'^2 + r^{-2}l(l+1)u^2 - 2uu'W]dr.$$

Now we have

$$2|uu'W| \leqq 2^{-1}u'^2 + 2u^2W^2.$$

Hence

$$0 \geqq \int_{r_p}^{r_{p+1}} (\tfrac{1}{2}u'^2 + r^{-2}l(l+1)u^2 - 2u^2W^2)dr$$

or, minorizing also the centrifugal energy term:

$$0 \geqq \int_{r_p}^{r_{p+1}} (u'^2 + r^{-2}l(l+1)u^2 - 4W^2u^2)dr. \tag{17}$$

Inequality (17) shows that if we solve the following Schrödinger equation

$$-w'' + r^{-2}l(l+1)w - 4W^2w = Ew, \tag{18}$$

in the interval $r_p < r < r_{p+1}$, with the boundary conditions $w(r_p) = w(r_{p+1}) = 0$, the ground state wave function w_{p+1} has a *negative* energy E_{p+1}, since there exists a trial function u which makes the energy *negative.*

Let us now call w_0 the solution of (18) at zero energy with the boundary condition $w_0(0) = 0$. We shall prove that w_0 has at least one zero in $]r_p, r_{p+1}[$. Indeed by combining the wave equations for w_{p+1} and w_0 we get

$$(w_{p+1}w_0' - w_{p+1}'w_0)\Big|_{r_p}^{r_{p+1}} = E_{p+1} \int_{r_p}^{r_{p+1}} w_{p+1}w_0 dr$$

or

$$w_0(r_{p+1})w_{p+1}'(r_{p+1}) - w_0(r_p)w_{p+1}'(r_p) = -E_{p+1} \int_{r_p}^{r_{p+1}} w_{p+1}w_0 dr. \tag{19}$$

Since w_{p+1} is the ground state wave function for the interval $r_p r_{p+1}$ it has no node and can be taken to be positive. Then $w_{p+1}'(r_{p+1}) < 0$ and $w_{p+1}'(r_p) > 0$. It is clear that Equation (19) is not consistent with a constant sign of w_0. Therefore w_0 has at least one zero in each interval $]r_p, r_{p+1}[$ including the interval $]0, r_1[$. Therefore the zero energy wave function for the potential $-4W^2$ has at least v_l nodes. The potential $-4W^2$ has at least as many bound states as the potential V:

$$v_l(V) \leqq v_l(-4W^2). \tag{20}$$

Let us repeat that from (4) and (5) it follows that $\int_0^\infty r(W(r))^2 dr$ converges and hence "classical" bounds can be used for the potential $-4(Wr))^2$. One can of course take the long list of existing bounds and make the substitution (20). Let us restrict ourselves to a few examples:

i) from the Bargmann bound we derive

$$v_l < 4(2l+1)^{-1} \int_0^\infty r(W(r))^2 dr \tag{21}$$

here we see that for $l=0$ we loose a factor 2 if we compare with inequality (12);

ii) more generally we can use the family of bounds proposed in [5]:

$$v_l < \frac{(p-1)^{p-1}\Gamma(2p)4^p}{p^p\Gamma^2(p)(2l+1)^{2p-1}} \int_0^\infty r^{2p-1} W^{2p}(r) dr \tag{22}$$

with $p \geqq 1$; this includes (21) as a limiting case;

iii) global bounds on the total number of bound states for all angular momenta, counted with the appropriate multiplicity factors, can be extended to this case:

$$N \leqq 16 \left[\int W^2 r^2 dr \int W^4 r^2 dr\right]^{1/2} \tag{23}$$

from the bound obtained by one of us (A.M.) [7],

$$N \leqq C \int |W|^3 r^2 dr \tag{24}$$

from the bound obtained by Rosenblum [8], Cwikel [9], and Lieb [10]. From Lieb's result one has $C \leqq 32\pi \times 0.116$.

It has been pointed out to us by Moulin-Combescure that the theorems stated by Rosenblum in [8], which apply to more general differential operators than the Schrödinger operator, allow one to get directly an inequality of the type (24). The advantage of our method, however, is that proofs are explicit.

3. Optimal Inequalities for Oscillating Potentials

In the previous section no attempt was made to obtain the best possible inequalities. In fact in inequality (17) we have minorized $(2l(l+1)/r^2)u^2$ by $(l(l+1)/r^2)u^2$. This could be avoided and would lead to reducing for instance the right-hand side of (21) by a factor $1/\sqrt{2}$. This, however, would not yet correspond to the best possible inequality.

Here we shall concentrate on inequalities involving $\int rW^2(r)dr$, i.e., the analogue of the Bargmann inequalities. However, exactly the same method can be applied to other cases.

In the $l=0$ case the inequality previously obtained [4] is the best possible one for the case of one bound state. Indeed take $V(r)=-c\delta(r-r_0)$, with $cr_0=1$. This produces a bound state at zero energy:

$$u(r)=r \qquad r\leqq r_0$$

$$u(r_0)=r_0$$

and

$$u'(r>r_0)-u'(r<r_0)=-Cr_0=-1\,.$$

Hence

$$u'(r)=0 \qquad r>r_0\,.$$

Then the Bargmann bound is saturated, $\int r|V(r)|dr=cr_0=1$, and the bound $2\int r(W(r))^2dr\leqq 1$ is also saturated for $2\int r(W(r))^2dr=2\int_0^{r_0} rc^2dr=(r_0c)^2=1$. In the case of ν bound states the inequality can also be shown to approach as close as one wishes to saturation. This has been done explicitly for instance by Elizalde [11] for the Bargmann bound. Let us, first for illustration, treat the case of two bound states. Take

$$-V(r)=(1+L^{-1})\delta(r-1)+\delta(r-L-L^2-1)/L^2\,.$$

The corresponding reduced wave function has a zero at $r=1+L$ and is constant for $r>1+L+L^2$. Then

$$\int r|V(r)|dr=1+L^{-1}+L^{-2}(L^2+L+1)=2+0(L^{-1})$$

as $L\to\infty$ we make the integral as close as we want to 2.

Similarly

$$\begin{aligned}2\int rW^2(r)dr&=2\left[\int_1^{1+L+L^2} r[L^{-2}]^2dr+\int_0^1 r[1+L^{-1}+L^{-2}]^2dr\right]\\&=2[L^{-2}(1+L+L^2)]^2\,,\end{aligned}$$

as close as we want to 2 for L big enough. Clearly that kind of example can be generalized.

Let us turn now to the case $l\neq 0$. In terms of W the energy of the ground state reads:

$$\begin{aligned}E&=\int(\dot u^2+l(l+1)r^{-2}u^2-2W(r)u\dot u)dr\\&\geqq\int(\dot u^2+l(l+1)r^{-2}u^2)dr-2\left[\int rW^2dr\int\dot u^2u^2r^{-1}dr\right]^{1/2}.\end{aligned}\tag{25}$$

Following the method of [5], we try to find

$$\mu=\operatorname{Inf}\left[\int(\dot u^2+l(l+1)r^{-2}u^2)dr\Big/\left[\int\dot u^2u^2r^{-1}dr\right]^{1/2}\right]\tag{26}$$

for all u's vanishing at $r=0$ and $r=\infty$. If $\mu\neq 0$ (which is already implicitly established in the previous section) we will be certain that there is no negative energy bound state if

$$\int rW^2(r)dr<(\mu/2)^2\,.\tag{27}$$

To find μ we shall follow again [5]. Define

$$\phi(z)=u(r)r^{-1/2}, \qquad z=\ln(r/r_0). \tag{28}$$

The scale r_0 is arbitrary. Then

$$\mu=\operatorname{Inf}\frac{\int_{-\infty}^{+\infty}(\dot\phi^2+\phi^2[4^{-1}+l(l+1)])dz}{\left[\int_{-\infty}^{+\infty}(\phi^2\dot\phi^2+\phi^4/4)dz\right]^{1/2}}. \tag{29}$$

Here we shall *admit* that the infimum is the solution of the variation equation for the right-hand side of (29). In [5], an explicit proof of that fact has been given for a similar minimization problem.

With

$$I=\int(\dot\phi^2+\phi^2(l+1/2)^2)dz, \tag{30}$$

$$J=\int(\dot\phi^2\phi^2+\phi^4/4)dz, \tag{31}$$

the variation equation is

$$\frac{-2\ddot\phi+2\phi(l+1/2)^2}{I}=\tfrac{1}{2}\frac{-2\ddot\phi\phi^2-2\dot\phi^2\phi+\phi^3}{J}. \tag{32}$$

By multiplication by ϕ and integration of both sides, we get, using $\phi(\infty)=0$

$$\frac{-\dot\phi^2+\phi^2(l+1/2)^2}{I}=\tfrac{1}{2}\frac{-\dot\phi^2\phi^2+\phi^4/4}{J}. \tag{33}$$

We can fix the scale of ϕ by fixing the ratio

$$I/2J=1. \tag{34}$$

Then (23) becomes

$$\dot\phi^2=4^{-1}\phi^2((2l+1)^2-\phi^2)/(1-\phi^2). \tag{35}$$

Since $\phi(\infty)=0$ this equation indicates that $|\phi|\leqq 1$. If $|\phi|<1$, Equation (32) indicates with normalization (34) that $\ddot\phi$ is finite. Therefore $\dot\phi$ cannot have a discontinuity and therefore cannot change its sign. $\dot\phi$ must, however, change sign once because $\phi(+\infty)=\phi(-\infty)=0$. We can now break the translation invariance with respect to z by deciding that $\phi(0)=1$, $\dot\phi<0$ for $z>0$, $\dot\phi>0$ for $z<0$. For $z>0$

$$\dot\phi=-2^{-1}(\phi^2((2l+1)^2-\phi^2)/(1-\phi^2))^{1/2} \tag{36}$$

the differential Equation (36) can be integrated giving z as a function of ϕ. This is not really necessary. Notice, however, that near $z=0$, for $l>0$,

$$\phi\sim 1-\text{const.}\,|z|^{2/3}. \tag{37}$$

It is sufficient to use (36) to compute directly

$$\int_{-\infty}^{+\infty}\dot\phi^2dz=2\int_0^{\infty}\dot\phi^2dz=2\int_0^1 d\phi\sqrt{\frac{\phi^2((2l+1)^2-\phi^2)}{4(1-\phi^2)}} \tag{38}$$

and

$$\int_{-\infty}^{+\infty} \phi^2 dz = 2\int_0^{\infty} \phi^2 dz = 2\int_0^1 d\phi \sqrt{\frac{4(1-\phi^2)\phi^2}{(2l+1)^2-\phi^2}}. \tag{39}$$

One finds in this way

$$I = (2l+1)[2l^2+2l+1] - 4(l(l+1))^2 \ln((l+1)/l). \tag{40}$$

With $I/2J \pm 1$ we get

$$\mu = \sqrt{2}[(2l+1)(2l^2+2l+1) - 4(l(l+1))^2 \ln((l+1)/l)]^{1/2} \tag{41}$$

and hence the condition for the absence of a bound state of angular momentum l is:

$$\int rW^2(r)dr < \tfrac{1}{2}[(2l+1)(2l^2+2l+1) - 4(l(l+1))^2 \ln((l+1)/l). \tag{42}$$

One can apply, of course, the same type of argument to the case of v_l bound states, use the fact that the zero energy wave function has v_l nodes, and that the infimum of the functional appearing in (17) for a function vanishing outside a finite interval is larger or equal to μ. Then one gets

$$v_l < \int_0^{\infty} r(W(r))^2 dr / \tfrac{1}{2}[(2l+1)(2l^2+2l+1) - 4(l(l+1))^2 \ln((l+1)/l)]. \tag{43}$$

For large l the denominator of (43) behaves like $4l/3$. This means that we have gained a factor 8/3 if we compare with (12).

Let us now discuss the question of the saturation of the bound, at least for one bound state. To get saturation the Schwarz inequality appearing in (16) must be saturated. This means

$$W(r) = \text{const}\ \dot{u}u/r. \tag{44}$$

Precisely the variation equation expressed in terms of u, with the variable r reads

$$-\ddot{u} + l(l+1)r^{-2}u = \text{const}((d/dr)\dot{u}u/r)u. \tag{45}$$

The only trouble is that the potential

$$V(r) = (d/dr)\dot{u}ur^{-1}, \quad \text{with} \quad u = r^{1/2}\phi(\ln r),$$

ϕ being the solution of Equation (35), is not acceptable because it is not integrable: $u \sim 1-(r-r_0|^{2/3}$, $\dot{u} \sim |r-r_0|^{-1/3}$, $\ddot{u} \sim |r-r_0|^{-4/3}$. However, one can perform a smearing procedure on ϕ:

$$\phi_\varepsilon(z) = \tfrac{3}{4}\int_{-1}^{+1} \phi(z+\varepsilon x)(1-x^2)dx \tag{46}$$

the smeared ϕ has bounded first and second derivatives. $\phi_\varepsilon(z) - \phi(z) \to 0$ uniformly for $\varepsilon \to 0$ and

$$\lim_{\varepsilon \to 0} \int_{-\infty}^{+\infty} dz(\dot{\phi}_\varepsilon^2 - \dot{\phi}^2) = 0 \tag{47}$$

because $(\dot{\phi})^2$ is integrable.

One can define

$$V_\varepsilon = (\ddot{u}_\varepsilon/u_\varepsilon) - l(l+1)/r^2$$

and

$$W_\varepsilon = -\int_r^\infty V_\varepsilon(r')dr'.$$

For $r > r_0$ it is clear that $\lim W_\varepsilon = W$ for $\varepsilon \to 0$. This is less clear but, however, true for $r < r_0$. Indeed

$$W_\varepsilon = (\dot{u}_\varepsilon/u_\varepsilon) - \int_r^\infty (\dot{u}_\varepsilon/u_\varepsilon)^2 dr' + l(l+1)/r$$

and since

$$\int (\dot{u}_\varepsilon/u_\varepsilon)^2 dr \to \int (\dot{u}/u)^2 dr, \qquad W_\varepsilon \to W$$

except at $r = r_0$.

In short,

i) $\int (\dot{\phi}_\varepsilon^2 + \phi_\varepsilon^2(l+\frac{1}{2}))^2 dz / [\int (\dot{\phi}_\varepsilon^2 \phi_\varepsilon + \phi_\varepsilon^4/4) dz]^{1/2}$

is as close as one wishes from the expression for $\varepsilon = 0$;

ii) $(\int W_\varepsilon u_\varepsilon \dot{u}_\varepsilon)^2$ is as close as one wishes from

$$\int r W_\varepsilon^2 dr \int u_\varepsilon^2 \dot{u}_\varepsilon^2 r^{-1} dr.$$

The potential V_ε has of course a completely different aspect from V, because it has an attractive well around $r = r_0$ which is physically essential to produce bound states. However, inequality (42) for the absence of bound states *cannot* be improved.

4. The Question of the Dependence on the Coupling Constant

Here, from now on we shall use a potential $gV(r)$. In the case of ordinary potentials there is the superficially paradoxical situation that the Bargmann bound $v_0 < g \int r |V(r) dr$ can be saturated though the asymptotic behaviour of v_0 for $g \to \infty$ is [12, 13]

$$v_0 \sim g^{1/2} \pi^{-1} \int V^-(r)^{1/2} dr, \tag{48}$$

where V^- designates the attractive part of the potential. To get (48) one has to assume either that $V(r)$ is piecewise monotonous which is what is done in [12] or that $\int_0^R |V(r)| dr$ is integrable (we assume fast decrease at infinity) as stated in [13].

For oscillating potentials the bound stated in Section 1 with the weakest coupling constant behaviour is the analogue of the Bargmann bound:

$$v_0 < 2g^2 \int_0^\infty r(W(r))^2 dr.$$

We may wonder if there is an analogue of (48). Since it is out of the question to impose integrability of $(W(r))^2$ at the origin which is too restrictive, we shall try to use monotony.

We work with the potential $-4W^2(r)$. This potential is *not* monotonous, otherwise $V(r)$ would be purely attractive and the convergence of $g\int_0^\infty W(r)dr$ would imply the convergence of $g\int_0^\infty r|V(r)|dr$. However, we have $\lim r|W(r)=0$. Hence

$$g|W(r)|<gC/r \tag{49}$$

because W is continuous and decreases anyway faster than $1/r$ at infinity. The bound is monotonous and we could try to use Calogero's inequality [14] valid for monotonous potentials

$$v_0<\tfrac{2}{\pi}g^{1/2}\int V(r)^{1/2}dr\,. \tag{50}$$

The trouble is that (49) leads to a divergent result.

Let us impose the slightly stronger condition

$$g|W(r)|<gCr^{-1}(\log(R/r))^{-\gamma}\,,\qquad \gamma>1\,,\qquad r\leqq R/2\,. \tag{51}$$

We also assume that

$$g|V(r)|<gcr^{-2-\varepsilon}$$

and, hence

$$g|W(r)|<gc'r^{-1-\varepsilon} \tag{52}$$

(this can be taken as our short-range condition). Since (51) and (52) are both *monotonous*, we get

$$v_0<g\left[c\int_0^{R/2} r^{-1}(\log(R/r))^{-\gamma}dr+c'\int_{R/2}^\infty r^{-1-\varepsilon}dr\right]+1\,, \tag{53}$$

where $+1$ accounts for the splitting of the interval 0∞ into two subintervals.

So by slightly strengthening condition (49), we manage to get a bound with the asymptotic behaviour $v\sim g$.

5. Concluding Remarks

In this paper we have tried to give an answer to the only question where oscillating potentials differ from classical regular potentials: that of the inequalities on bound state energies, for which the classical bounds diverge. If one is only interested in qualitative information, the inequality $v_l(V)<v_l(-4W^2)$ is amply sufficient. One may of course question the physical relevance of such potentials, but the fact is that this class of potentials appears in a very natural way in the inverse problem of reconstruction of potentials from phase shifts [1]. Also these results may be useful for other fields of mathematical physics where Sturm-Liouville equations with oscillating coefficients appear.

Acknowledgements. We thank Mrs. Moulin-Combescure for stimulating discussions. One of us (A.M.) acknowledges the hospitality of the Laboratoire de Physique Théorique et Particules Elémentaires, Orsay, where this investigation was started, and the other (K.C.) the Theoretical Physics Division of CERN where it was completed.

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Communicated by W. Hunziker

Received December 13, 1976