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SOME SIMPLE CONDITIONS ON BOUND STATES OF SCHRÖDINGER OPERATORS IN DIMENSION d ≥ 3

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Introduction

A substantial part of the information provided to us by the quantum theory stems from various non-relativistic potential models. Hence all methods for treating bound states of Schrödinger operators are of physical interest, in particular, those devised for estimating the number, multiplicities and location of the corresponding eigenvalues. There are different types of such estimates. Some of them are, in fact, receipts for iterative calculating of the eigenvalues, say, the Rayleigh-Ritz variational method combined with a suitable lower bound - see, e.g., the papers /1,2/ for further references. They can yield highly accurate results, but they require certain tedious procedures, in particular, solving large systems of algebraic equations.

Here we shall be concerned with another type of estimates which yield relatively poorer results but in a much simpler way, mostly via suitable integrals of the potential involved. Various methods of this type have been elaborated during the last three decades - for a review and bibliography see Ref.3, especially Section XIII.3 . Notice that the merit of such methods is not only to give a quick orientation about character of $\sigma_{disc}(H)$ for a given Schrödinger operator $H = -\Delta + V$. They can be useful also in the cases when the above mentioned quantitative methods are difficult to be applied, or when the exact answer is not actually needed. As an example, recall the well-known problem of stability of matter, where one looks just for a suitable lower bound to the ground-state energy of the appropriate many-particle Hamiltonian /4/.

Recently, Rosen /5/ used a Sobolev inequality to get a necessary condition for existence of bound states of the Schrödinger operator $H = -\Delta + V$ on $\mathcal{H} = L^2(\mathbb{R}^3)$. By the same method, he deduced a lower bound to the set of all bound-state energies, i.e., to the ground-state energy of H . These results are not new from the most part (see Refs.33,34 , and the concluding remarks), but their proofs are attractive being simple and straightforward. They are expressed through the potential V alone, or more exactly, in terms of integrals of certain powers of $|V|$. Another attractive feature is that no symmetry of the potential is required. On the other hand, there are some drawbacks too. First of all, the results of Ref.5 are confined to the Schrödinger operators in the three-dimensional configuration space. Another restrictive feature is that convergence of the mentioned integrals demands V to decay rapidly enough at infinity. In this way, the results do not apply to many physically important cases : long-range forces such as the Coulomb one, confining potentials, etc.

It is the aim of this paper to show that these restrictions can be removed. We shall be concerned with the Schrödinger operators $H = -\Delta + V$ on $\mathcal{H} = L^2(\mathbb{R}^d)$, where d is any dimension ≥ 3. The assumptions about the potential are the following :

(a) H is self-adjoint on its natural domain $D(-\Delta) \cap D(V)$,

(b) the needed integrals (cf.(2.4),(2.7) below) converge for the appropriate values of the parameters ε, γ.

The first hypothesis is rather implicit, of course, but there are many powerful self-adjointness criteria which may be used to check it - we refer particularly to Chapter X of the monograph[3]. In fact, one may require H to be essentially self-adjoint only, provided we know that its eigenvectors belong to the domain of essential self-adjointness (see also the concluding remarks).

The paper is organized as follows. First we recall briefly a few facts concerning the Sobolev inequalities which are essential for the method. In Section 2 we derive our main results, namely a necessary condition for existence of a bound state of H with an energy less than a given ε, and a related lower bound for the ground-state energy. In order to appreciate the obtained necessary condition, we compare it in Section 3 with some other known conditions (see Refs.6-9, or Ref.3, Theorem XIII.9) for several simple spherically symmetric potentials. The next two sections contain the discussion of two examples that illustrate how our results generalize and improve those of Ref.5. They concern the d-dimensional hydrogen-like atom and the d-dimensional harmonic oscillator, $d \geq 3$. In both cases, we obtain lower bounds to the ground state energy which become remarkably tight for large values of d. The final section contains a few remarks, in particular, one concerning the relation of our necessary condition to Cwikel-Lieb-Rosenbljum theorem, and another one devoted to the Schrödinger operators with complex potentials. The results of the paper were announced in Ref.30.

1. A Preliminary : Sobolev Inequalities

There is a wide variety of inequalities bearing this name because of their common origin in the paper[10]. Their most standard form can be found, e.g., in Ref.3, Section IX. Starting from it, one can derive another set of inequalities (Ref.11, Section V.2), which are often called alternately Sobolev imbedding theorems. They yield a bound on the L^q-norm of a given function $\psi: \mathbb{R}^d \to \mathbb{C}$ by means of the L^p-norm of $|\nabla\psi|$, the length of its gradient,

$$\|\psi\|_q = \left(\int_{\mathbb{R}^d} |\psi(x)|^q dx\right)^{1/q} \leq C_{p,d}\left(\int_{\mathbb{R}^d} |(\nabla\psi)(x)|^p dx\right)^{1/p} , \qquad (1.1)$$

where $-q^{-1}+p^{-1} = d^{-1}$ and $C_{p,d}$ is a constant independent of ψ (here and in the following, we write dx instead of d^dx). For our purposes, the case $p = 2$ is important, where

$$q = \frac{2d}{d-2} \qquad (1.2)$$

(so one requires $d \geq 3$) and (1.1) may be rewritten as

$$\|\nabla\psi\|_2 \geq K_d \|\psi\|_q \quad . \qquad (1.3)$$

The best constant for the inequality (1.1) was found by Talenti[12]; for $p = 2$ his result gives

$$K_d^2 = \pi d(d-2) \left[2^{d-1}\pi^{-1/2}\,\Gamma\left(\frac{d+1}{2}\right)\right]^{-2/d} \quad . \qquad (1.4)$$

Particularly in the three-dimensional case we have the value

$$K_3^2 = 3(\pi/2)^{4/3} , \qquad (1.5)$$

which was suggested earlier by Rosen[13]. Notice also that ψ saturating (1.3) is of the form[12]

$$\psi(x) = \text{const} . (x^2+\alpha^2)^{1-d/2} ; \qquad (1.6)$$

it does not belong to $L^2(\mathbb{R}^d)$ for $d = 3,4$, but it may be approximated by L^2-functions.

2. The Main Results

Let us look first for a necessary condition on H to have an eigenvalue below a given energy ε. Equivalently, one may ask whether the operator $H_\varepsilon \equiv H - \varepsilon$ has a negative eigenvalue, so it is useful to introduce the shifted potential $V(\varepsilon,.) = V(.) - \varepsilon$. For our purposes, the (positively taken) negative part

$$V_-(\varepsilon,x) := \max\{0, \varepsilon - V(x)\} \tag{2.1}$$

will be essential ; similarly we denote $V_+(\varepsilon,x) = \max\{0, V(x)-\varepsilon\}$.

First we take $\varepsilon = 0$ and abbreviate $V_\pm(0,x) = V_\pm(x)$. If H has a negative eigenvalue E corresponding to a unit vector $\psi \in D(H) = D(-\Delta) \cap D(V)$, then it holds

$$\|\nabla\psi\|_2^2 + \int_{\mathbb{R}^d} V(x)\,|\psi(x)|^2\,dx = E < 0$$

so (1.3) together with (2.1) and the Hölder inequality give

$$K_d^2\|\psi\|_q^2 \le \|\nabla\psi\|_2^2 < -\int_{\mathbb{R}^d} V_+(x)\,|\psi(x)|^2\,dx + \int_{\mathbb{R}^d} V_-(x)\,|\psi(x)|^2\,dx \le$$
$$\le \int_{\mathbb{R}^d} V_-(x)\,|\psi(x)|^2\,dx \le \left(\int_{\mathbb{R}^d} V_-(x)^a\,dx\right)^{1/a} \|\psi\|_{2b}^2 , \tag{2.2}$$

where $a^{-1} + b^{-1} = 1$. Choosing $2b = q$, we can eliminate $\|\psi\|_q^2$ from the resulting inequality. The relation (1.2) gives then $a = q/(q-2) = \frac{1}{2}d$, so the sought condition reads

$$\left(\int_{\mathbb{R}^d} V_-(x)^{d/2}\,dx\right)^{2/d} > K_d^2 . \tag{2.3}$$

Applying now the same argument to the operator $H_\varepsilon = -\Delta + V(\varepsilon,.)$, we arrive at the following assertion :

<u>Theorem 1</u> : Assume (a) and $V_-(\varepsilon,.) \in L^{d/2}(\mathbb{R}^d)$ for a given ε. The condition

$$\int_{\mathbb{R}^d} V_-(\varepsilon,x)^{d/2}\,dx > K_d^d = \frac{\pi^{1/2}(\pi d(d-2))^{d/2}}{2^{d-1}\,\Gamma\left(\frac{d+1}{2}\right)} \tag{2.4}$$

is necessary for the operator H to have an eigenvalue below ε.

Apart from the extension to the dimensions $d > 3$, there are two (standard) improvements here comparing to Ref.5 . The

first one concerns the middle inequality in the above chain (2.2), which replaces the more rough estimate by $\int_{\mathbb{R}^d} |V(x)|\,|\psi(x)|^2\,dx$. The other is the eventual shift on ε. In combination, they lead to the condition (2.4), which is sensitive to the values of the potential below the chosen ε only. In this way, one is able to eliminate the influence of a slowly decaying tail of V or its growth at infinity.

At a glance, the above considerations may seem to be slightly academical, because the existence of bound states represents a real problem just for the short-range forces. One should realize, however, that the condition (2.4) can provide at the same time a lower bound to the point spectrum of H, i.e., to its ground-state energy E_0. This is so, because the lhs of (2.4) is strictly monotonous with respect to ε (with exception of those parts of $\mathbb{R}$, where it is equal eventually to 0 or ∞). Thus we get

$$E_0 > \varepsilon_0 , \tag{2.5a}$$

where ε_0 is the solution to the equation

$$\int_{\mathbb{R}^d} V_-(\varepsilon,x)^{d/2}\,dx = K_d^d ; \tag{2.5b}$$

if it exists, the monotonicity implies its uniqueness.

Now we are going to modify the method of the above proof to derive a more general bound on E_0 in terms of the integrals

$$\int_{\mathbb{R}^d} V_-(\varepsilon,x)^{\gamma d/2}\,dx , \quad \gamma > 1 . \tag{2.6}$$

<u>Theorem 2</u> : Suppose that (a) is valid and the integrals (2.6) are finite for some ε and $\gamma > 1$, then any eigenvalue E of H fulfils the inequality

$$E \geq \varepsilon - (1-\gamma^{-1})\left[\gamma^{-d/2} K_d^{-d} \int_{\mathbb{R}^d} V_-(\varepsilon,x)^{\gamma d/2}\,dx\right]^{2/d(\gamma-1)} . \tag{2.7}$$

In particular, this is true for the ground-state energy E_0.

<u>Proof</u> : One can again consider the case $\varepsilon = 0$ only, the argument for the general case being obtained by replacement of E and $V_-(x)$ by $E-\varepsilon$ and $V_-(\varepsilon,x)$, respectively. Let ψ be a normalized eigenvector, $\|\psi\|_2 = 1$, corresponding to E, then in analogy with (2.2) we can write

$$E = \|\nabla\psi\|_2^2 + \int_{\mathbb{R}^d} V(x)\,|\psi(x)|^2\,dx \;\geq$$

$$\geq K_d^2\,\|\psi\|_q^2 - \int_{\mathbb{R}^d} V_-(x)\,|\psi(x)|^2\,dx \quad . \tag{2.8a}$$

Further we estimate the last term from below using twice the Hölder inequality

$$\int_{\mathbb{R}^d} V_-(x)\,|\psi(x)|^2\,dx \leq \left(\int_{\mathbb{R}^d} V_-(x)^a\,dx\right)^{1/a} \|\psi\|_{ce}^{c/b}\,\|\psi\|_{(2b-c)f}^{(2b-c)/b} \,, \tag{2.8b}$$

where, of course, $a^{-1}+b^{-1}=1$ and $e^{-1}+f^{-1}=1$, and c is some number from $(0,2b)$. We want to choose the parameters in such a way that $ce=2$, so the second factor on the rhs can be removed in view of the normalization, and at the same time, $(2b-c)f=q$. It is easy to see that these requirements are fulfilled if we set

$$a = \tfrac{1}{2}\gamma d \;, \quad b = \frac{\gamma d}{\gamma d-2} \;, \quad c = \frac{2d(\gamma-1)}{\gamma d-2} \;,$$
$$e = \frac{\gamma d-2}{d(\gamma-1)} \;, \quad f = \frac{\gamma d-2}{d-2} \;. \tag{2.9}$$

The relations (2.8),(2.9) together imply

$$E \geq K_d^2\,\|\psi\|_q^2 - \left(\int_{\mathbb{R}^d} V_-(x)^{\gamma d/2}\,dx\right)^{2/\gamma d} \|\psi\|_q^{2/\gamma} \quad .$$

The last step consist of minimizing the rhs with respect to $\|\psi\|_q$, which yields

$$E \geq -(1-\gamma^{-1})\left(\gamma^{-d/2}\,K_d^{-d}\int_{\mathbb{R}^d} V_-(x)^{\gamma d/2}\,dx\right)^{2/d(\gamma-1)} \,,$$

i.e., the desired result. ∎

Remark : Suppose that the integrals (2.6) converge for $\gamma=1$ too in a sufficiently large interval of ε's , and that they are right continuous at this point. Denoting as $f(\varepsilon,\gamma)$ the rhs of (2.7), one can easily calculate the limit

$$\lim_{\gamma\to 1+} f(\varepsilon,\gamma) = \begin{cases} \varepsilon & \dots \quad \int_{\mathbb{R}^d} V_-(\varepsilon,x)^{d/2}\,dx \leq K_d^d \\ -\infty & \dots \quad \int_{\mathbb{R}^d} V_-(\varepsilon,x)^{d/2}\,dx > K_d^d \end{cases}$$

so the bound (2.7) leads back to (2.5) under the stated assumptions.

3. Comparison with Some Other Necessary Conditions for $d=3$

Most of the known necessary conditions for existence of bound states concern spherically symmetric potentials in the three-dimensional configuration space. Let the function $V:\mathbb{R}_+\to\mathbb{R}$ describe such a potential. The inequality (2.4) with $\varepsilon=0$ can be in that case rewritten as

$$\int_0^\infty V_-(r)^{3/2}\,r^2\,dr > \frac{3^{3/2}\pi}{16} = 1.02026 \quad . \tag{3.1}$$

This result should be compared, e.g., with the following conditions (valid for the spherically symmetric potentials from $(R+L^\infty_\varepsilon)(\mathbb{R}^3)$ – see Ref.3, Theorem XIII.9) :

(a) JPB-condition/6,7/ :

$$\int_0^\infty |V(r)|\,r\,dr > 1 \quad , \tag{3.2}$$

(b) Calogero condition/8/ :

$$\int_0^\infty |V(r)|^{1/2}\,dr > \frac{\pi}{2} \quad , \tag{3.3}$$

which is valid if V is non-positive and its modulus is non-increasing with respect to r ,

(c) GMGT-condition /9/ :

$$\int_0^\infty |V(r)|^p\,r^{2p-1}\,dr > \frac{p^p\,\Gamma(p)^2}{(p-1)^{p-1}\,\Gamma(2p)} \tag{3.4}$$

valid for each $p>1$.

To be concrete, consider a few simple spherically symmetric potentials, which fulfil obviously the assumptions of Theorem 1 :

(i) the rectangular well :

$$V(r) = \begin{cases} -V_0 & \dots \quad r\leq a \\ 0 & \dots \quad r>a \,, \end{cases} \tag{3.5}$$

(ii) the exponential well :

$$V(r) = -V_0\,e^{-r/a} \quad , \tag{3.6}$$

(iii) Yukawa potential :

$$V(r) = -V_0 a \frac{e^{-r/a}}{r} \quad . \tag{3.7}$$

The results yielded by the conditions (3.1)-(3.4) are listed in Table I below. In particular, the values referring to the GMGT-con-

Table I : Comparison of various necessary and sufficient conditions for existence of a bound state in the potentials (3.5)-(3.7).

	Necessary conditions				Necessary and sufficient condition c)	Variational sufficient condition d)
	(3.1)	JPB	Calogero	GMGT b)		
rectangular well $V_0a^2 >$	2.10809	2	2.46740 a)	2.35927 p=1.175	2.46740	2.94121
exponential well $V_0a^2 >$	1.43469	1	0.61685	1.43833 p=1.455	1.44580	1.6875
Yukawa potential $V_0a^2 >$	1.64767	1	0.39270	1.66427 p=1.675	1.680	2

a) In this case the potential is not strictly monotonous except at one point, and (3.3) yields the exact value $(\pi/2)^2$.

b) We list simultaneously the optimal value of p .

c) It is easy to find in the first two cases (see Ref.14, Section 2.4.3 ; Ref.15, Section 12.3), the value for Yukawa potential is taken from Ref.9, or Ref.16, Problem 4.49 .

d) One usually looks for the conditions under which $(\psi, H\psi)$ can be negative with a suitable trial function ψ (Ref.16, Problem 4.48 ; Ref.17, Problem 72). This yields a sufficient condition if only the essential spectrum of H is bound to $[0,\infty)$, what is certainly true for the potentials under consideration (see, e.g., Ref.3, Section XIII.4).

dition are obtained by numerical optimalization over p . For comparison, we present also the exact values, and the rough sufficient condition obtained from the variational argument with the exponential trial function, $\psi(x) = 2\alpha^{3/2} e^{-\alpha r}$. The purpose of these examples is, of course, rather illustrative. Apart from a higher accuracy and one slight correction, most of the values listed here can be found already in Ref.9, where also the Gaussian-shaped well is treated.

In all these examples, the potentials are non-positive so $V_- = |V|$. Actually, the modulus may be replaced by V_- in the conditions (3.2)-(3.4) even if V assumes positive values. This follows from the minimax principle (see Ref.3, proof of Theorem XIII.9) : if H has a bound state, then the same is true for $H_- = -\Delta + V_-$ (cf. also Ref.21, Proposition 4). Thus (3.1) turns out to be a particular case of the GMGT-condition corresponding to $p = \frac{3}{2}$ (notice that the results achieved with (3.1) are rather good, when $p = \frac{3}{2}$ is close to the optimal value). On the other hand, the condition (3.1) has the advantage that it represents a specification of the much more general result expressed by Theorem 1 .

4. d-Dimensional Kepler Problem

Here we shall treat the first of two mentioned d-dimensional examples. The Hamiltonian H on $L^2(\mathbb{R}^d)$ will be

$$H = -\Delta + \frac{2\alpha}{r} \quad , \tag{4.1}$$

where $r = \left(\sum_{j=1}^{d} x_j^2\right)^{1/2}$ and α is a positive constant ; H is self-adjoint on $D(-\Delta)$, because the potential belongs to $(L^p + L^\infty)(\mathbb{R}^d)$ for all $p < d$, and therefore for any fixed $p \in (\frac{1}{2}d, d)$ (cf.Ref.3, Section X.2). The ground-state energy of this operator is known[18] to be

$$E_0 = -\frac{4\alpha^2}{(d-1)^2} \quad . \tag{4.2}$$

Let us apply now our Theorem 2 . The integrals (2.6) exist in this case for each $\varepsilon < 0$ and $1 < \gamma < 2$. Since the potential is spherically symmetric, we have

$$\int_{\mathbb{R}^d} V_-(\varepsilon,x)^{\gamma d/2}\, dx = \frac{2\pi^{d/2}}{\Gamma(d/2)} \int_0^{2\alpha|\varepsilon|^{-1}} \left(\frac{2\alpha}{r} - |\varepsilon|\right)^{\gamma d/2} r^{d-1}\, dr \quad . \tag{4.3}$$

The last integral is easily evaluated (Ref.19, 3.131, 8.335) so the inequality (2.7) can be rewritten with the help of (1.4) as

$$E \geq -|\varepsilon| - (1-\gamma^{-1}) \left[(2\alpha)^d (\gamma d(d-2))^{-d/2} \times \frac{\Gamma(1+\frac{\gamma d}{2})\,\Gamma(d-\frac{\gamma d}{2})}{\Gamma(\frac{d}{2})\,\Gamma(1+\frac{d}{2})} \right]^{2/d(\gamma-1)} |\varepsilon|^{(\gamma-2)/(\gamma-1)} . \tag{4.4}$$

Next one has to maximize the rhs with respect to $|\varepsilon|$; it yields

$$E \geq -\frac{4\alpha^2}{d(d-2)}\, \gamma^{-\gamma} (2-\gamma)^{\gamma-2} \left[\frac{\Gamma(1+\frac{\gamma d}{2})\,\Gamma(d-\frac{\gamma d}{2})}{\Gamma(\frac{d}{2})\Gamma(1+\frac{d}{2})} \right]^{2/d} . \tag{4.5}$$

Denoting the rhs as $E_0(\gamma)$, we see easily that $\lim_{\gamma \to 2-} E_0(\gamma) = -\infty$. An orientative analysis suggests the function $E_0(.)$ is presumably decreasing in the whole interval $(1,2)$. In such a case, the best lower bound following from (4.5) is

$$E \geq \lim_{\gamma \to 1+} E_0(\gamma) = -\frac{4\alpha^2}{d(d-2)} . \tag{4.6}$$

In particular, for $d=3$ the last inequality gives $E_0 \geq -\frac{4}{3}\alpha^2$, the known bound to the hydrogen ground-state energy $E_0 = -\alpha^2$ (cf. Ref.4, Eq.(9)). It is a remarkable fact that the analogous bound becomes better with increasing the dimension d ; the relations (4.2) and (4.6) give

$$\lim_{\gamma \to 1+} \frac{E_0(\gamma)}{E_0} = \frac{(d-1)^2}{d(d-2)} \tag{4.7}$$

so the relative error of the estimate is $\lesssim d^{-2}$ for large d .

5. d-Dimensional Harmonic Oscillator

In this example, the Hamiltonian H on $L^2(\mathbb{R}^d)$ is of the form

$$H = -\Delta + \omega^2 r^2 , \tag{5.1}$$

where again $r^2 = \sum_{j=1}^{d} x_j^2$ and $\omega > 0$. The ground-state energy of H is

$$E_0 = \omega d . \tag{5.2}$$

As we have already claimed, the estimates (2.7) work in spite of the fact that the potential is growing. Check of the assumption (a) is easy (see Ref.20, Proposition 1). The integrals (2.6) converge for all ε and $\gamma > 1$ (in fact, for $\gamma > -2/d$ too). In analogy with (4.3), we have for a positive ε the expression

$$\int_{\mathbb{R}^d} V_-(\varepsilon,x)^{\gamma d/2}\, dx = \frac{2\pi^{d/2}}{\Gamma(d/2)} \int_0^{\varepsilon^{1/2}/\omega} (\varepsilon - \omega^2 r^2)^{\gamma d/2}\, r^{d-1}\, dr , \tag{5.3}$$

so after evaluation of the integral (Ref.19, 3.191) and substitution to (2.7) we get

$$E \geq \varepsilon - (1-\gamma^{-1}) \left[\frac{1}{2}\pi^{-1/2} (\pi d(d-2))^{-d/2} \left(\frac{2}{\omega}\right)^d \times \frac{\Gamma(\frac{d+1}{2})\,\Gamma(1+\frac{\gamma d}{2})}{\Gamma\left(1+\frac{(\gamma+1)d}{2}\right)} \right]^{2/d(\gamma-1)} \varepsilon^{(\gamma+2)/(\gamma-1)} . \tag{5.4}$$

Taking the maximal value of the rhs with respect to ε , we obtain the inequality

$$E \geq \omega (d(d-2))^{1/2} \gamma^{\gamma/2} (\gamma+1)^{-(\gamma+1)/2} \left[\frac{2\pi^{1/2}\,\Gamma\left(1+\frac{(\gamma+1)d}{2}\right)}{\Gamma(\frac{d+1}{2})\,\Gamma(1+\frac{\gamma d}{2})} \right]^{1/d} . \tag{5.5}$$

On the basis of numerical tests, we conjecture that the rhs (denoted as $E_0(\gamma)$) is again decreasing with respect to γ , this time with the finite limit

$$\lim_{\gamma \to \infty} E_0(\gamma) = \omega d \left(\frac{d-2}{2e}\right)^{1/2} \left(\frac{1}{2}\pi^{-1/2}\,\Gamma\left(\frac{d+1}{2}\right) \right)^{-1/d} .$$

The best lower bound following from (5.5) is then

$$E \geq \lim_{\gamma \to 1+} E_0(\gamma) = 2^{1/d} (d(d-2))^{1/2} \omega . \tag{5.6}$$

Table II

The lower bound to the ground-state energy (5.2) from (5.6).

d	$\lim_{\gamma \to 1+} E_0(\gamma)$	d	$\lim_{\gamma \to 1+} E_0(\gamma)$
3	2.18225 ω	50	49.6737 ω
4	3.36359 ω	100	99.6835 ω
5	4.44889 ω	10^3	999.692 ω
10	9.58623 ω	10^6	999999.69 ω

As in the previous example, the estimate to the ground-state energy (5.2) becomes closer with the increasing d, the relative error being $< d^{-1}$. This is illustrated by the table.

6. Remarks

1. The interest to various qualitative methods of analyzing the discrete spectrum of the Schrödinger operators is not ceasing – for other recent results see, e.g., Refs. 22-24.

2. The term "bound state" used in the introduction might seem inexact, since no multiplicity requirements are made in Theorems 1,2. In most practical cases, however, the eventual differences between $\sigma_{disc}(H)$ and $\sigma_{point}(H)$ are not important : either we know location of the essential spectrum (Ref.3, Sections XIII.4,5) and we are interested in the eigenvalues that lay outside it, or even $\sigma_{ess}(H)$ is empty, say, by the Molchanov criterion/25/ or some similar reason.

3. Among various bounds to the number $N(\varepsilon,V)$ of the eigenvalues (counted with multiplicities) of a Schrödinger operator $H=-\Delta+V$ on $L^2(\mathbb{R}^d)$, $d\geq 3$, that lay not above a given ε, the probably most general is given by the Cwikel-Lieb-Rosenbljum theorem (see Refs. 21, 26-28, or Ref.3, Theorem XIII.12, or Ref.29, Theorem 9.3). In our notation, it reads

$$N(\varepsilon,V)\leq a_d\int_{\mathbb{R}^d} V_-(\varepsilon,x)^{d/2}\,dx\ , \tag{6.1}$$

where a_d is some constant independent of V and ε. Since the rhs is strictly monotonous with respect to ε, the inequality becomes sharp if we consider only the eigenvalues located below ε. In particular, we have

$$a_d\int_{\mathbb{R}^d} V_-(\varepsilon,x)^{d/2}\,dx > 1 \tag{6.2}$$

if only H has an eigenvalue below ε. Hence we obtained the condition (2.4) up to the value of the constant. Furthermore, we have the inequality

$$a_d\geq a_d^S=\frac{2^{d-1}\,\Gamma\left(\frac{d+1}{2}\right)}{\pi^{1/2}(\pi d(d-2))^{d/2}}\ , \tag{6.3}$$

which is derived from (6.1) by a Sobolev-inequality argument sketched in Ref.29, Section III.9 (for an upper bound to a_d see Ref.21). By Lieb-Thirring conjecture, (6.3) becomes equality for $d\leq 7$, in which case $a_d=K_d^{-d}$ and (2.4) turns out to be a consequence of (6.1).

On the other hand, a_d is known to be strictly larger than a_d^S for $d\geq 8$; then our Theorem 1 strengthens the necessary condition (6.2) following from the CLR-theorem. The improvement is substantial for higher dimensions, because $a_d\geq a_d^c$ (Ref.29, Section III.9) and $a_d^c/a_d^S\to\infty$ as $d\to\infty$.

4. It should be mentioned that the GMGT-condition for $p\geq\frac{3}{2}$ may be formulated without the requirement of spherical symmetry of the potential. A result of this type with $p=\frac{3}{2}$ was derived first by Faris (see Ref.9).

5. As for Theorem 2, let us first notice that a more general inequality was derived in Ref.33 (see Eq.(25) of this paper and also Ref.34). However, the μ-dependent factor that multiplies the integral is given only implicitly there ; it is not obvious whether it would coincide with that of (2.7).

6. Another problem related to the bound (2.7) is the following. In the above two examples, the best lower bounds are presumably achieved for $\mu\to 1+$. In Ref.5, Rosen treated the exponential well (3.6) by means of (2.7) with $\varepsilon=0$; he obtained the best lower bound for $\mu\approx 1.7262\,(V_0a^2)^{1/3}$ if $V_0a^2\gg 1$. A numerical test suggests that this bound cannot be probably improved by choosing a negative ε. In the case of the rectangular well (3.5), a simple calculation shows that (2.7) yields the optimal bound for a non-zero ε independently of μ. The question about existence of a potential for which the rhs of (2.7) has a strict maximum for some values ε,μ that lay inside the allowed strip is left open.

7. As we have already mentioned, the self-adjointness assumption is not actually needed. The considerations of Section 2 require only that the eigenvectors of H belong simultaneously to the domains of both $-\Delta$ and V. In fact, the results are partly preserved even if the potential V is not real-valued. Such generalized Schrödinger operators can be of direct physical interest if they are maximal dissipative, because then they may provide models of dissipative systems (cf.Ref.31, or Ref.32, Chapter 4). Consider an operator of this type, $H=-\Delta+U$ on $L^2(\mathbb{R}^d)$ corresponding to a complex potential $U=V-iW$, and suppose that H is maximal dissipative on $D(-\Delta)\cap D(U)$. The relation analogous to the first equality in (2.8a) shows then that the proofs can be easily adapted to yield relations between the real part of an eigenvalue E of H and the real part V of the potential U. Hence under the assumption (b), the inequality (2.4) expresses a necessary condition for H to have an eigenvalue with $\mathrm{Re}\,E<\varepsilon$, and $\mathrm{Re}\,E$ is bounded from below by the rhs of (2.7).

8. As an illustration, consider the operator H corresponding to the spherically symmetric d-dimensional damped harmonic oscillator described by the complex potential $U : U(x) = \Omega^2 r^2$, where $\Omega = \omega - i\nu$ with $0 < \nu \leq \omega$ (see Ref.20, and Ref.32, Section 6.2). Since the requirement of maximal dissipativity is fulfilled and $V(x) = (\omega^2 - \nu^2)r^2$, we obtain in analogy with (5.6) the inequality

$$\mathrm{Re}\, E \geq 2^{1/d}(d(d-2))^{1/2}(\omega^2 - \nu^2)^{1/2} , \qquad (6.4)$$

which holds particularly for the real part of the "ground-state" eigenvalue $E_0 = (\omega - i\nu)d$. In distinction to the real case, however, the bound (6.4) is no longer asymptotically exact : the ratio of its rhs to ωd tends to $(1-\nu^2/\omega^2)^{1/2} < 1$ as $d \to \infty$.

References

1 Hill R.N., J.Math.Phys., 1980, v.21, pp.2182-2192.

2 Hornby P.G., Barber M.N., J.Phys.A, 1983, v.16, pp.3291-3311.

3 Reed M. and Simon B., Methods of Modern Mathematical Physics, II.Fourier Analysis, Self-Adjointness, IV.Analysis of Operators, Academic Press, New York, 1975, 1978.

4 Lieb E.H., Rev.Mod.Phys., 1976, v.48, pp.553-569.

5 Rosen G., Phys.Rev.Lett.,1982, v.49, pp.1885-1887.

6 Jost R. and Pais A., Phys.Rev., 1951, v.82, pp.840-850.

7 Bargmann V., Proc.Nat.Acad.Sci.USA, 1952, v.38, pp.961-966.

8 Calogero F., Commun.Math.Phys.,1965, v.1, pp.80-88.

9 Glaser V., Martin A., Grösse H. and Thirring W., A Family of Optimal Conditions for the Absence of Bound States in a Potential, in "Studies in Mathematical Physics : Essays in Honor of V.Bargmann" (E.Lieb et al., eds.), pp.169-194, Princeton University Press, 1976.

10 Sobolev S.L., Mat.Sbornik, 1938, v.46, pp.471-497 (in Russian).

11 Stein E.M., Singular Integrals and Differentiability Properties of Functions, Princeton University Press, 1970.

12 Talenti G., Annali Mat.Pura et Appl.,1976, v.110, pp.353-372.

13 Rosen G., SIAM J. of Appl.Math., 1971, v.21, pp.30-32.

14 Formánek J., Introduction to Quantum Theory (in Czech), SPN, Prague, 1974.

15 Morse P.M. and Feshbach H., Methods of Theoretical Physics, McGraw-Hill Book Co, New York, 1953.

16 Galickii V.M., Karnakov B.M. and Kogan V.I., Problems in Quantum Mechanics (in Russian), Nauka, Moscow, 1981.

17 Flügge S., Practical Quantum Mechanics, Vol.I, Springer-Verlag, Berlin, 1971.

18 Bargmann V., Helv.Phys.Acta,1972, v.45, pp.249-257.

19 Gradshtein I.S. and Ryzhik I.M., Tables of Integrals, Series, Sums and Products (in Russian), Nauka, Moscow, 1971.

20. Exner P., J.Math.Phys.,1983, v.24, pp.1129-1135.

21 Lieb E.H., The Number of Bound States of One-Body Schrödinger Operators and the Weyl Problem, in "Geometry of the Laplace Operator" (R.Osserman, A.Weinstein, eds.), Proceedings of Symposia in Pure Mathematics, v.36, pp.241-252, American Mathematical Society, Providence, Rhode Island, 1980.

22 Exner P., Generalized Bargmann Inequalities, Preprint JINR E2-12373, Dubna, 1979 ; to appear in Rep.Math.Phys.

23 Requardt M., Some New Estimates on Eigenfunctions, Eigenvalues, Expectation Values, Number of Bound States in Schrödinger Theory, Preprint, University of Göttingen, 1983.

24 Chadan K. and Grösse H., New Bounds on Number of Bound States, Preprint CERN TH-3380, 1983.

25 Molchanov A.M., Trudy Mosk.Mat.Obshchestva, 1953, v.2, pp.169--200.

26 Rosenbljum G.V., Dokl.Akad.Nauk SSSR, 1972, v.202, pp.1012-1015.

27 Lieb E.H., Bull.Amer.Math.Soc.,1976, v.82, pp.751-753.

28 Cwikel M., Ann.of Math.,1977, v.106, pp.93-102.

29 Simon B., Functional Integration and Quantum Physics, Academic Press, New York, 1979.

30 Exner P., Improved Rosen's Conditions on Bound States of Schrödinger Operators, Preprint JINR E2-84-49, Dubna, 1984.

31 Blank J., Exner P. and Havlíček M., Czech.J.Phys.B, 1979, v.29, pp.1325-1341.

32 Exner P., Open Quantum Systems and Feynman Integrals, D.Reidel, Dordrecht, to appear.

33 Glaser V., Grosse H. and Martin A., Commun.Math.Phys.,1978, v.59, pp.197-212.

34 Glaser V. and Martin A., Lett.N.Cim.,1983, v.36, pp.519-520.

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Экснер П.

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Некоторые простые условия на связанные состояния операторов Шредингера размерности $d \geq 3$

Пользуясь неравенствами Соболева, мы выводим необходимое условие для существования связанных состояний ниже заданной энергии для оператора Шредингера $H = -\Delta + V$ на $L^2(R^d)$, $d \geq 3$, вместе с оценкой снизу на энергию основного состояния оператора H. Это обобщает некоторые недавно полученные результаты для случаев размерности $d > 3$ и для потенциалов, которые не должны быстро убывать на бесконечности. Приводится сравнение с другими известными необходимыми условиями. Обсуждаются примеры d-размерного водородоподобного атома и d-размерного гармонического осциллятора. В обоих случаях полученная оценка снизу на энергию основного состояния становится довольно тесной для больших значений d.

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Exner P.

E2-84-51

Some Simple Conditions on Bound States of Schrödinger Operators in Dimension $d \geq 3$

A necessary condition for existence of bound states below a given energy of a Schrödinger operator $H = -\Delta + V$ on $L^2(R^d)$, $d \geq 3$, together with a lower bound to the ground-state energy of H are derived using the Sobolev inequalities. It generalizes some recent results to the dimensions $d > 3$ and to the potentials that are not necessarily rapidly decreasing. Comparison to other known necessary conditions is given. The examples of the d-dimensional hydrogen-like atom and the d-dimensional harmonic oscillator are discussed.In both of them,the bound to the ground-state energy becomes remarkably tight for large values of d.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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