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SOME NORM BOUNDS AND QUADRATIC FORM INEQUALITIES FOR SCHRÖDINGER OPERATORS. II

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1. INTRODUCTION

In this paper we discuss questions such as the boundedness of the operator $V(H_0 + V)^{-1}$ when V is a potential on an open region $\Omega \subseteq \mathbf{R}^N$, and H_0 is minus the Laplacian with Dirichlet boundary conditions. Because we treat rather singular potentials V it is necessary to use quadratic form techniques systematically, and to pay careful attention to domain questions. Although many of the results in [4] are superceded by the present paper, we draw attention in Appendix 1 to a technical gap in [4] which makes several proofs here more devious than one might have thought necessary.

The initial reason for the estimates in this paper was the desire to obtain a comparison theorem of the form

$$\|(H_0 + V_1)^{-1} - (H_0 + V_2)^{-1}\| \leqslant c\|V_1^{-1} - V_2^{-1}\|$$

where V_i are both strictly positive potentials, which may have very strong local singularities. Such a bound is given in Section 4, and will be used in a subsequent paper to study double well Schrödinger operators. However, in the course of the work, we discovered a number of quite different applications of Theorem 6 (our main result), which we decided to include in this paper.

In order to apply Theorem 6 effectively it is necessary to find suitable potentials X such that $0 \leqslant X \leqslant H_0$, where H_0 is minus the Laplacian in $L^2(\Omega)$ with Dirichlet boundary conditions. This is actually an entirely independent problem, which we discuss in Section 5. An immediate consequence of these calculations is to give a new lower bound to the spectrum of H_0 in terms of a quantity μ which we call the quasi-inradius of Ω because of its similarity to the ordinary inradius, known to be of relevance to this problem if $N = 2$. This lower bound is given and discussed in Section 6.

We start by assuming that Ω is an open region in $\mathbf{R}^N$, and impose no regularity properties on its boundary. We identify $L^2(\Omega)$ with the set of functions in $L^2(\mathbf{R}^N)$ which vanish almost everywhere outside Ω. We denote by D_i the usual partial differentiation operators, which are the closures of those operators initially defined on $C_c^\infty(\Omega)$. We then define H_0 to be the form closure of the operator $-\Delta$ initially defined on $C_c^\infty(\Omega)$. Equivalently we might define H_0 by

$$\langle H_0^{1/2}f, H_0^{1/2}f\rangle = \sum_{i=1}^{N} \langle D_i f, D_i f\rangle$$

with

$$\mathrm{Quad}(H_0) \equiv \mathrm{Dom}(H_0^{1/2}) = \bigcap_{i=1}^{N} \mathrm{Dom}(D_i).$$

The form of H_0 is a restriction of the form of minus the Laplacian of the whole of $\mathbf{R}^N$, to a suitable subdomain which is dense in $L^2(\Omega)$.

We next define the class $\mathscr{V}$ of potentials V which we will ultimately consider. We say $V \in \mathscr{V}$ if $V \in L^1_{\mathrm{loc}}(\Omega)$ and the negative part V_- of V satisfies a form bound

$$V_- \leqslant aH_0 + b$$

for some $0 \leqslant a < 1$ and $0 \leqslant b < \infty$. The form sum $H_0 \dot{+} V$ may then be defined in two stages by

$$H_0 \dot{+} V = (H_0 - V_-) \dot{+} V_+$$

with

$$\mathrm{Quad}(H_0 \dot{+} V) = \mathrm{Quad}(H_0 - V_-) \cap \mathrm{Quad}\, V_+ =$$

$$= \mathrm{Quad}(H_0) \cap \mathrm{Quad}\, V_+ \supseteq C_c^\infty(\Omega).$$

We shall use the fact that $H_0 \dot{+} V$ is a semi-bounded self-adjoint operator, with the further property that if $\lambda > b$ then $(H_0 \dot{+} V + \lambda)^{-1}$ is positivity preserving. By this we mean that $0 \leqslant f \in L^2(\Omega)$ implies

$$0 \leqslant (H_0 \dot{+} V + \lambda)^{-1} f$$

or equivalently that the integral kernel of the operator is pointwise non-negative. Moreover if $V \leqslant V'$ then the integral kernel of $(H_0 \dot{+} V + \lambda)^{-1}$ dominates that of $(H_0 \dot{+} V' + \lambda)^{-1}$ pointwise. These results may all be deduced from the Trotter product formula.

We denote by $C_b^1(\Omega)$ the space of continuously differentiable functions f on Ω which are bounded together with all their first order partial derivatives. The following lemma provides reassurance that some expressions in Lemma 2 are meaningful.

LEMMA 1. *If* $W \in C_b^1(\Omega)$ *then*

$$W(\mathrm{Quad}(H_0)) \subseteq \mathrm{Quad}(H_0).$$

Proof. If $f \in C_c^\infty(\Omega)$ then $Wf \in \mathrm{Dom}(D_i)$ for all i and

$$D_i(Wf) = W_i f + W(D_i f)$$

where $W_i = \frac{\partial W}{\partial x_i}$. Thus

$$\|D_i(Wf)\|^2 \leqslant 2\|W_i f\|^2 + 2\|W(D_i f)\|^2 \leqslant$$

$$\leqslant 2\|W_i\|_\infty^2 \|f\|^2 + 2\|W\|_\infty^2 \|D_i f\|^2.$$

Putting

$$|||f||| = (\|f\|^2 + \sum \|D_i f\|^2)^{1/2}$$

we deduce that there exists $c < \infty$ such that

$$|||Wf||| \leqslant c|||f|||$$

for all $f \in C_c^\infty(\Omega)$. But $\mathrm{Quad}(H_0)$ is the completion of $C_c^\infty(\Omega)$ for the norm $|||\cdot|||$, so W defines a bounded operator of the completion into itself.

LEMMA 2. *Suppose* V *is bounded and*

$$0 < c \leqslant W \in C_b^1(\Omega).$$

Then

$$\|(H_0 + V)f\|^2 \geqslant 2\mu\|H_0^{1/2} W^{1/2} f\|^2 + \tag{1}$$

$$+ \left\langle \left(2\mu WV - \mu^2 W^2 - \frac{\mu\|\nabla W\|^2}{2W}\right) f, f \right\rangle$$

for all $f \in \mathrm{Dom}(H_0)$ *and all* $\mu \geqslant 0$.

Proof. We first note that since V is bounded

$$\mathrm{Dom}(H_0 + V) = \mathrm{Dom}(H_0) \subseteq \mathrm{Quad}(H_0) = \bigcap_{i=1}^{N} \mathrm{Dom}(D_i).$$

Since

$$0 \leqslant \langle (H_0 + V - \mu W)f, (H_0 + V - \mu W)f \rangle =$$

$$= \langle (H_0 + V)f, (H_0 + V)f \rangle - \mu\langle Wf, (H_0 + V)f \rangle -$$

$$- \mu\langle (H_0 + V)f, Wf \rangle + \mu^2 \langle Wf, Wf \rangle$$

we see that

$$\|(H_0 + V)f\|^2 \geq 2\mu\langle VWf,f\rangle - \mu^2\langle W^2f,f\rangle + \mu\langle Wf, H_0f\rangle + \mu\langle H_0f, Wf\rangle = \tag{2}$$

$$= 2\mu\langle VWf,f\rangle - \mu^2\langle W^2f,f\rangle + \mu \sum_{i=1}^{N} [\langle D_iWf, D_if\rangle + \langle D_i f, D_iWf\rangle].$$

Next observe that f and Wf lie in $\mathrm{Dom}(D_i)$ by Lemma 1. Moreover W has a strictly positive lower bound, and this implies $W^{1/2} \in C_b^1(\Omega)$. It follows that

$$\langle D_iWf,D_if\rangle = \left\langle\left(\frac{W_i}{2W^{1/2}} + W^{1/2}D_i\right) W^{1/2}f, D_if\right\rangle =$$

$$= \left\langle\left(\frac{W_i}{2W^{1/2}} + D_iW^{1/2}\right)f, W^{1/2}D_if\right\rangle =$$

$$= \left\langle\left(\frac{W_i}{2W^{1/2}} + D_iW^{1/2}\right)f, \left(D_iW^{1/2} - \frac{W_i}{2W^{1/2}}\right)f\right\rangle.$$

Adding this to its conjugate we obtain

$$\langle D_iWf, D_if\rangle + \langle D_if, D_iWf\rangle = 2\langle D_iW^{1/2}f, D_iW^{1/2}f\rangle - \left\langle\frac{W_i^2}{2W}f,f\right\rangle.$$

The lemma follows by substituting this equality (due to Glimm and Jaffe [5]) into (2).

The following corollary is a technically restricted version of our main theorem.

COROLLARY 3. *Suppose that V is bounded and that the potential X on Ω satisfies*

$$0 \leq X \leq H_0 \tag{3}$$

in the sense of quadratic forms. Suppose that $W \in C_b^1(\Omega)$ satisfies

$$0 < c \leq W \leq V + X \tag{4}$$

for some c, and

$$\|\nabla W\|^2 \leq 4\alpha^2W^2(V + X) \tag{5}$$

for some $0 < \alpha < 1$. Then

$$(1 - \alpha^2)\|W^{1/2}(V + X)^{1/2}f\| \leq \|(H_0 + V)f\| \tag{6}$$

for all $f \in \mathrm{Dom}(H_0 + V)$.

Proof. Substituting the bounds (3), (4) and (5) into Lemma 2 yields

$$\|(H_0 + V)f\|^2 \geq 2\mu\|X^{1/2}W^{1/2}f\|^2 + \langle(2\mu WV - \mu^2W^2 - 2\mu\alpha^2W(V + X))f, f\rangle \geq$$

$$\geq \langle\mu(2 - \mu - 2\alpha^2)\, W(V + X)f,f\rangle.$$

If $0 < \alpha < 1$ then the optimum choice of μ is $\mu = 1 - \alpha^2$, and this yields

$$\|(H_0 + V)f\|^2 \geqslant (1 - \alpha^2)^2 \langle W(V + X)f, f\rangle$$

as stated.

Our remaining task is to weaken the conditions on V and W in the above corollary.

LEMMA 4. *The result of Corollary 3 remains valid if one assumes that $V \in \mathscr{V}$ instead of assuming that V is bounded.*

Proof. The assumptions on W ensure that there is a finite constant b such that

$$\|\nabla W\|^2 \leqslant 4\alpha^2 W^2 b,$$

$$0 \leqslant W \leqslant b.$$

Combining this with (4) and (5) we see that if

$$V_{b,n} = \begin{cases} -n & \text{if } V(x) \leqslant -n, \\ V(x) & \text{if } -n < V(x) < b, \\ b & \text{if } V(x) \geqslant b, \end{cases}$$

then

$$0 < c \leqslant W \leqslant V_{b,n} + X,$$

$$\|\nabla W\|^2 \leqslant 4\alpha^2 W^2 (V_{b,n} + X).$$

Applying Corollary 3 we deduce that

$$(1 - \alpha^2)\|W^{1/2}(V_{b,n} + X)^{1/2} f\| \leqslant \|(H_0 + V_{b,n})f\|$$

for all $f \in \mathrm{Dom}(H_0 + V_{b,n})$, or equivalently

$$\|W^{1/2}(V_{b,n} + X)^{1/2}(H_0 + V_{b,n} + \lambda)^{-1}\| \leqslant (1 - \alpha^2)^{-1}$$

for all $\lambda > 0$. The operator on the left-hand side has a non-negative integral kernel and pointwise domination and monotonicity arguments lead successively to

$$\|W^{1/2}(V_{b,\infty} + X)^{1/2}(H_0 + V_{b,n} + \lambda)^{-1}\| \leqslant (1 - \alpha^2)^{-1},$$

$$\|W^{1/2}(V_{b,\infty} + X)^{1/2}(H_0 + V_{b,\infty} + \lambda)^{-1}\| \leqslant (1 - \alpha^2)^{-1},$$

$$\|W^{1/2}(V_{b,\infty} + X)^{1/2}(H_0 + V + \lambda)^{-1}\| \leqslant (1 - \alpha^2)^{-1},$$

$$\|W^{1/2}(V + X)^{1/2}(H_0 + V + \lambda)^{-1}\| \leqslant (1 - \alpha^2)^{-1}.$$

This final bound is equivalent to the statement of the lemma.

We finally define the class $\mathscr{G}$ of potentials W in which we are interested. We first require that $W:\Omega \to (0, \infty]$ is continuous and that

$$S := \{x \in \Omega : W(x) = \infty\}$$

is a relatively closed null set. We also require that W is continuously differentiable on $\Omega \setminus S$ and that for all $c > 0$ there exists $C < \infty$ such that

$$W(x) \leqslant C \quad \text{implies} \quad \|\nabla W(x)\| \leqslant c.$$

Equivalently if $x_n \in \Omega \setminus S$ and $\|\nabla W(x_n)\| \to \infty$ then $W(x_n) \to \infty$. For an even more general class than $\mathscr{G}$ see Appendix 2.

LEMMA 5. *Let* $W_n = F_n(W)$ *where* $W \in \mathscr{G}$ *and* $F_n:[0, \infty) \to [0, \infty)$ *is defined by*

$$F_n(t) := \begin{cases} t(1 + t/4n)^{-2} & \text{if } 0 \leqslant t \leqslant 4n, \\ n & \text{if } 4n < t < \infty. \end{cases}$$

Then W_n *is continuously differentiable and increases monotonically to* W *as* $n \to \infty$. *Moreover*

$$0 \leqslant W_n \leqslant n, \tag{7}$$

$$0 \leqslant \|\nabla W_n\|/W_n \leqslant \|\nabla W\|/W, \tag{8}$$

$$0 \leqslant \|\nabla W_n\| \leqslant c_n < \infty, \tag{9}$$

for some sequence c_n, *at every point of* Ω.

Proof. A direct computation shows that

$$0 \leqslant tF_n'(t) \leqslant F_n(t) \tag{10}$$

for all n and t, and that $F_n(t)$ increases monotonically to t as $n \to \infty$. Since

$$\frac{\|\nabla W_n\|}{W_n} = \frac{WF_n'(W)}{F_n(W)} \frac{\|\nabla W\|}{W}$$

we see that (8) follows from (10). The other statements of the lemma are easy to check.

The following theorem is the main technical result of the paper. In [4] we treated only the case $W = V$ and $X = 0$, but it turns out that one can get better bounds in many circumstances by more careful choices of W and X. One suitable choice of X, depending on the shape of Ω, is given in Section 5.

We remark that a proof of Theorem 6 might also be based upon suitably strong pointwise bounds on the non-negative integral kernel of $(H_0 \dot{+} V)^{-1}$. For related estimates of this type see [11], where, however, strong local singularities of V are not permitted, because H_0 is taken to be defined on the whole of $\mathbf{R}^N$.

For an even more general version of Theorem 6 see Appendix 2.

THEOREM 6. *Let $V \in \mathscr{V}$, $W \in \mathscr{G}$ and let the potential X on Ω satisfy*

$$0 \leqslant X \leqslant H_0$$

in the sense of quadratic forms. Suppose that

$$0 \leqslant W \leqslant V + X$$

and

$$\|\nabla W\|^2 \leqslant 4\alpha^2 W^2 (V + X)$$

for some $0 < \alpha < 1$. Then

$$(1 - \alpha^2) \, \|W^{1/2}(V + X)^{1/2} f\| \leqslant \|(H_0 \dot{+} V) f\|$$

for all $f \in \mathrm{Dom}(H_0 \dot{+} V)$.

Proof. If $0 < \mu < \lambda < \infty$ and

$$W_n = F_n(W + \mu)$$

then $W_n \in C_b^\infty(\Omega)$ and

$$0 < \mu \leqslant W_n \leqslant W + \mu \leqslant (V + \lambda) + X.$$

Also

$$\frac{\|\nabla W_n\|}{W_n} \leqslant \frac{\|\nabla W\|}{W + \mu}$$

by Lemma 5, so

$$\frac{\|\nabla W_n\|^2}{W_n^2} \leqslant 4\alpha^2 \frac{W^2}{(W + \mu)^2} (V + X) \leqslant 4\alpha^2 \{(V + \lambda) + X\}.$$

We deduce from Lemma 4 that

$$(1 - \alpha^2) \, \|W_n^{1/2}(V + \lambda + X)^{1/2} f\| \leqslant \|(H_0 \dot{+} V + \lambda) f\|$$

for all $f \in \mathrm{Dom}(H_0 \dot{+} V)$. Letting $n \to \infty$ we deduce that

$$(1 - \alpha^2) \, \|W^{1/2}(V + X)^{1/2} f\| \leqslant$$

$$\leqslant (1 - \alpha^2) \, \|(W + \mu)^{1/2}(V + \lambda + X)^{1/2} f\| \leqslant \|(H_0 \dot{+} V \dot{+} \lambda) f\|.$$

The result now follows by letting $\lambda \to 0$.

The following simple special case of Theorem 6 is sometimes useful.

COROLLARY 7. *Let $V \in \mathcal{V}$, $W \in \mathcal{G}$ and let*

$$0 \leqslant X \leqslant H_0$$

in the sense of quadratic forms. Suppose that

$$0 \leqslant W \leqslant V + X$$

and

$$\|\nabla W\| \leqslant cW$$

for some $c \geqslant 1$. Then

$$\|W(H_0 \dotplus V + 1)^{-1}\| \leqslant 2c.$$

Proof. We have

$$\|\nabla(c^{-2}W)\|^2 \leqslant c^{-2}W^2 \leqslant c^{-2}W(V + X) \leqslant$$

$$\leqslant \frac{1}{2}(c^{-2}W + 1)^2((V + 1) + X).$$

Therefore Theorem 6 applies with $\alpha^2 = 1/8$, V replaced by $(V + 1)$ and W replaced by $(c^{-2}W + 1)$. We conclude that

$$\frac{7}{8}\|Wf\| \leqslant \frac{7}{8}c\|(c^{-2}W + 1)^{1/2}(V + X + 1)^{1/2}f\| \leqslant$$

$$\leqslant c\|(H_0 \dotplus V + 1)f\|$$

for all $f \in \mathrm{Dom}(H_0 \dotplus V)$, and this implies the stated result.

2. LOCAL SINGULARITIES OF SCHRÖDINGER OPERATORS

As our first application of Theorem 6, we consider the operator $H = H_0 \dotplus V$ in $L^2(\mathbf{R}^3)$, where $V(x) = \frac{c}{x^\alpha}$ for some $c > 0$ and $\alpha > 0$. In [4] we showed that

$$\|V(H + 1)^{-1}\| < \infty \tag{11}$$

if $\alpha < 3/2$ or $\alpha > 2$, and also for $\alpha = 2$ if $c > 3/2$. Simon [12] subsequently showed that if $\alpha = 2$ then (11) holds if and only if $c > 3/4$, and he proved that the minimum values of a in the estimate

$$\|Vf\| \leqslant a\|Hf\|$$

is $a = c/(c - 3/4)$. His method of proof depended both on the spherical symmetry of V and on the fact that it is homogeneous of degree -2. Using Theorem 6, we are now able to rederive this optimum bound.

THEOREM 8. *If* $\alpha = 2$ *and* $N = 3$ *and* $c > 3/4$ *then*

$$\|Vf\| \leqslant \frac{c}{c - 3/4} \|Hf\|$$

for all $f \in \mathrm{Dom}(H)$.

Proof. We apply Theorem 6 with $X = \dfrac{1}{4x^2}$ and $W = (c + 1/4)/x^2$, so that $W = V + X$. We find that

$$\|\nabla W\| = 2(c + 1/4)/x^3$$

so

$$\|\nabla W\|^2 = 4\alpha^2 W^2 (V + X)^2$$

provided

$$4(c + 1/4)^2 = 4\alpha^2 (c + 1/4)^2 (c + 1/4)$$

which simplifies to

$$\alpha^2 = (c + 1/4)^{-1}.$$

Thus the condition $0 < \alpha < 1$ necessitates $c > 3/4$. Theorem 6 implies that

$$\{1 - (c + 1/4)^{-1}\}(c + 1/4)\left\| \frac{1}{x^2} f \right\| \leqslant \|Hf\|$$

which in turn implies that

$$\|Vf\| = c\left\| \frac{1}{x^2} f \right\| \leqslant \frac{c}{c - 3/4} \|Hf\|.$$

Theorem 6 is easily able to yield a variety of related results, of which the following is a sample.

THEOREM 9. *If in the notation of this section we have* $\alpha = 2$ *and* $N = 3$ *and* $-1/4 < c \leqslant 3/4$ *then*

$$\| |Q|^{-1-\beta} (H + 1)^{-1} \| \leqslant (c + 1/4 - \beta^2)^{-1}$$

for any β *such that* $0 < \beta^2 < c + 1/4$, *where* Q *is the position operator on* $L^2(\mathbf{R}^3)$.

Proof. We put $X = 1/4Q^2$, $V = 1 + c/Q^2$ and

$$W = (c + 1/4)/Q^2\beta$$

so that

$$0 \leqslant W \leqslant (c + 1/4)(1 + Q^{-2}) \leqslant$$

$$\leqslant 1 + (c + 1/4)/Q^2 = V + X.$$

Also

$$\|\nabla W\|^2 = \{2\beta(c + 1/4)\,|Q|^{-2\beta-1}\}^2 \leqslant$$

$$\leqslant 4\beta^2 W^2/Q^2 \leqslant \frac{4\beta^2}{c + 1/4} W^2(V + X).$$

If we now put

$$\alpha^2 = \beta^2/(c + 1/4)$$

then all the conditions of Theorem 6 are satisfied provided

$$0 < \beta^2 < c + 1/4.$$

The theorem follows once one notes that

$$W^{1/2}(V + X)^{1/2} \geqslant (c + 1/4)\,|Q|^{-1-\beta}.$$

NOTE. We conjecture that the power of $|Q|$ in this theorem and the upper bound $(c + 1/4)^{1/2}$ on β are the best possible, but have no similar confidence in the estimate of the norm.

As yet another application of Theorem 6 we consider the following generalization of Theorem 8.

THEOREM 10. *Let Ω be an open subset of $\mathbf{R}^N$ and let $V = c\,d(x)^{-2}$, where $c > 1$ and $d: \Omega \to (0, \infty)$ is continuously differentiable with $\|\nabla d(x)\| \leqslant 1$ for all $x \in \Omega$. Then*

$$\|Vf\| \leqslant \frac{c}{c - 1} \|(H_0 \dot{+} V)f\|$$

for all $f \in \mathrm{Dom}(H_0)$.

Proof. We put $X = 0$ and $W = V$ in Theorem 6. Then

$$\|\nabla W\| \leqslant 2c\, d(x)^{-3}$$

so

$$\|\nabla W\|^2 \leqslant 4c^{-1}W^2V$$

and Theorem 6 is applicable with $\alpha^2 = c^{-1}$, if $c > 1$.

NOTE. The choice

$$d(x) = \operatorname{dist}(x, c\Omega) = \min\{\|x - y\| : y \notin \Omega\}$$

satisfies $\|\nabla d(x)\| \leqslant 1$, provided d is continuously differentiable. According to Appendix 2 an even more general version of Theorem 6 enables one to cope with the cases where this function $d(x)$ is not differentiable everywhere. One might actually take $d(x)$ to be the distance from any closed subset S of $\mathbf{R}^n$, and in this case it would be interesting to determine how the optimal constant in the bound depends on S.

3. CONNECTIONS WITH THE AGMON METRIC

If $\lambda : \Omega \to (0, \infty)$ is a positive continuous function then one may define a "distance" $d(x, y)$ between two points $x, y \in \Omega$ by

$$d_\lambda(x, y) = \inf_\gamma \int_0^1 \lambda(\gamma(t))^{1/2} \|\gamma'(t)\| \, dt$$

where the infimum is over all smooth paths γ in Ω with $\gamma(0) = x$ and $\gamma(1) = y$. It was observed by Agmon [1, 2] and others [3, 13] that many asymptotic properties of eigenfunctions of $H_0 \dotplus V$ can be expressed in terms of this metric, provided

$$0 \leqslant \lambda \leqslant H_0 \dotplus V$$

in the sense of quadratic forms.

A close connection between our ideas and the Agmon metric is established by the following theorem. It would be interesting to obtain a deeper understanding of this result. The regularity assumptions on λ and W can surely be greatly relaxed, at the cost of a more complicated proof (see Appendix 2).

THEOREM 11. *Suppose that $0 \leqslant X \leqslant H_0$ and that $\lambda = V + X$ is strictly positive and continuous. Then a continuously differentiable function $W : \Omega \to (0, \infty)$ satisfies*

$$\|\nabla W(x)\|^2 \leqslant 4\alpha^2 W(x)^2 (V(x) + X(x)) \tag{12}$$

for all $x \in \Omega$ *if and only if*

$$W(y) \leqslant W(x) \exp[2\alpha\, d_\lambda(x, y)]$$

for all $x, y \in \Omega$.

Proof. It is elementary that

$$\|\nabla \log W(x)\| = \|\nabla W(x)\|/W(x)$$

so (12) is equivalent to

$$\|\nabla \log W(x)\|^2 \leqslant 4\alpha^2 \lambda(x)$$

or to

$$\|\nabla \log W(x)\| \leqslant 2\alpha\, \lambda(x)^{1/2}.$$

This in turn is equivalent to

$$|\log W(y) - \log W(x)| \leqslant 2\alpha \int_0^1 \lambda(\gamma(t))^{1/2} \|\gamma'(t)\|\, dt$$

for all paths from x to y within Ω.

4. COMPARISON OF RESOLVENTS

If $H_0 \dot{+} V_i$ are two Schrödinger operators on $L^2(\Omega)$, $\Omega \subseteq \mathbf{R}^N$, then a formal calculation yields

$$(H_0 \dot{+} V_1 + \lambda)^{-1} - (H_0 \dot{+} V_2 + \lambda)^{-1} = A^* BC \tag{13}$$

for all suitable λ, where

$$A = (V_1 + \lambda)(H_0 \dot{+} V_1 + \lambda)^{-1},$$

$$B = (V_1 + \lambda)^{-1} - (V_2 + \lambda)^{-1},$$

$$C = (V_2 + \lambda)(H_0 \dot{+} V_2 + \lambda)^{-1}.$$

This calculation is certainly correct if V_1 and V_2 are bounded, but in general it is not obvious that it is correct even if A, B, C are all bounded operators. This point was missed in [4], so that the proofs of certain theorems there have gaps. We show in this section that one *does* have the bound

$$\|(H_0 \dot{+} V_1 + \lambda)^{-1} - (H_0 \dot{+} V_2 + \lambda)^{-1}\| \leqslant \|A\|\, \|B\|\, \|C\|$$

under conditions on V_1 and V_2 of the type considered in this paper. Since we are interested in situations where B is bounded, we assume that $V_1 \geqslant 0$ and $V_2 \geqslant 0$ throughout this section.

We handle A and C by the following special case of Theorem 6.

LEMMA 12. *Let* $0 < \lambda \leqslant V \in \mathscr{G}$ *and let the potential* X *on* $\Omega \subseteq \mathbf{R}^N$ *satisfy the quadratic form bound*

$$0 \leqslant X \leqslant H_0.$$

Suppose that

$$\|\nabla V\|^2 \leqslant 4\alpha^2 V^2(V + X)$$

for some $0 < \alpha < 1$. *Then*

$$\|V(H_0 \dotplus V)^{-1}\| \leqslant (1 - \alpha^2)^{-1}.$$

Proof. Putting $V = W$ in Theorem 6, we obtain

$$\|Vf\| \leqslant \|V^{1/2}(V + X)^{1/2} f\| \leqslant$$

$$\leqslant (1 - \alpha^2)^{-1} \|(H_0 \dotplus V)f\|$$

for all $f \in \mathrm{Dom}(H_0 \dotplus V)$. The inclusion of the condition $\lambda > 0$ in the hypotheses ensures that $H_0 \dotplus V$ has a bounded inverse.

THEOREM 13. *Suppose that* $0 < \lambda_i \leqslant V_i \in \mathscr{G}$, *that* $0 \leqslant X \leqslant H_0$ *and that*

$$\|\nabla V_i\|^2 \leqslant 4\alpha_i^2 V_i^2(V_i + X)$$

for some $0 < \alpha_i < 1$. *Then*

$$\|(H_0 \dotplus V_1)^{-1} - (H_0 \dotplus V_2)^{-1}\| \leqslant (1 - \alpha_1^2)^{-1}(1 - \alpha_2^2)^{-1} \|V_1^{-1} - V_2^{-1}\|.$$

Proof. Instead of trying to justify the formula (13) by careful consideration of domain questions, we prove the result by a truncation procedure.

If $F_n(t)$ is defined as in Lemma 5 then a direct computation shows that

$$0 \leqslant t^3 F_n'(t)^2 \leqslant F_n(t)^3$$

for all $0 \leqslant t < \infty$. If we put

$$V_{i,n} = F_n(V_i)$$

then

$$\nabla V_{i,n} = F_n'(V_i) \nabla V_i$$

so

$$\|\nabla V_{i,n}\|^2 \leqslant V_i^{-3} V_{i,n}^3 4\alpha_i^2 V_i^2 (V_i + X) = 4\alpha_i^2 V_{i,n}^3 (1 + X/V_i) \leqslant$$

$$\leqslant 4\alpha_i^2 V_{i,n}^3 (1 + X/V_{i,n}) = 4\alpha_i^2 V_{i,n}^2 (V_{i,n} + X).$$

We deduce from Lemma 12 that

$$\|V_{i,n}(H_0 + V_{i,n})^{-1}\| \leqslant (1 - \alpha_i^2)^{-1}.$$

Since $V_{i,n}$ are bounded, the argument at the start of this section leads without trouble to the estimate

$$\|(H_0 + V_{1,n})^{-1} - (H_0 + V_{2,n})^{-1}\| \leqslant (1 - \alpha_1^2)^{-1}(1 - \alpha_2^2)^{-1} \|V_{1,n}^{-1} - V_{2,n}^{-1}\|.$$

Since the operators on the LHS converge strongly as $n \to \infty$, and the operators on the RHS converge in norm as $n \to \infty$, the theorem follows.

In the following variant of this theorem, which yields an even stronger bound if V_1 and V_2 only differ where X is very large, we do not require V_1 and V_2 to be positive.

THEOREM 14. *Suppose that X is bounded, $0 \leqslant X \leqslant H_0$, and that $W_i = X + V_i \in \mathscr{G}$ satisfy $0 < \lambda_i \leqslant W_i$ and*

$$\|\nabla W_i\|^2 \leqslant 4\alpha_i^2 W_i^3$$

where $0 < \alpha_i < 1$. Then

$$\|(H_0 + V_1)^{-1} - (H_0 + V_2)^{-1}\| \leqslant (1 - \alpha_1^2)^{-1}(1 - \alpha_2^2)^{-1} \|(X + V_1)^{-1} - (X + V_2)^{-1}\|.$$

Proof. This is straightforward if V_i are bounded, since

$$(H_0 + V_1)^{-1} - (H_0 + V_2)^{-1} = A^* BC$$

where

$$A = W_1(H_0 + V_1)^{-1},$$

$$C = W_2(H_0 + V_2)^{-1},$$

$$B = W_1^{-1}(V_2 - V_1)W_2^{-1} = W_1^{-1} - W_2^{-1}$$

and

$$\|W_i(H_0 + V_i)^{-1}\| \leqslant (1 - \alpha_i^2)^{-1}$$

by Theorem 6. The general case follows by putting $V_{i,n} = W_{i,n} - X$ where $W_{i,n} = F_n(W_i)$, and letting $n \to \infty$ as before.

NOTE. The condition that X is bounded was only imposed so that $V_{i,n}$ would be bounded, and can probably be eliminated with a more complicated argument.

5. BOUNDS ON THE DIRICHLET LAPLACIAN

In order to make Theorem 6 as powerful as possible, it is desirable to obtain a variety of potential X on $\mathbf{R}^N$ such that

$$0 \leqslant X \leqslant H_0.$$

Since

$$X(x) = \frac{1}{4} \|x - a\|^{-2}$$

is such a potential for any $a \in \mathbf{R}^3$ and any $\Omega \subseteq \mathbf{R}^3$, we see that there does not exist a largest such potential, and indeed that the set of such potentials is not directed upwards. One might nevertheless look for potentials X which are simple in form, and useful in appropriate situations. The potential X which we shall obtain gives quantitative expression to the idea that the Dirichlet boundary conditions force H_0 to be "large" near the boundary of Ω. We start with a slight variation of a classical inequality.

LEMMA 15. *If $f : [a, b] \to \mathbf{C}$ is continuously differentiable with $f(a) = f(b) = 0$ then*

$$\int_a^b \frac{|f(x)|^2}{4d(x)^2} \mathrm{d}x \leqslant \int_a^b |f'(x)|^2 \mathrm{d}x$$

where

$$d(x) = \min\{|x - a|, |x - b|\}.$$

Proof. One applies the standard uncertainty principle estimate [10, p. 169] to each half-interval separately.

Now let us consider a general open subregion Ω of $\mathbf{R}^N$. Given $u \in \mathbf{R}^N$ with $\|u\| = 1$ and $x \in \Omega$ we define

$$d_u(x) = \min\{|t| : x + tu \notin \Omega\}.$$

If $e(1), \ldots, e(N)$ is a given orthonormal basis of $\mathbf{R}^N$ we define

$$d_i(x) = d_{e(i)}(x).$$

LEMMA 16. *If $f \in C_c^\infty(\Omega)$ then*

$$\sum_{i=1}^N \int_\Omega \frac{|f(x)|^2}{4d_i(x)^2} \mathrm{d}^N x \leqslant \langle H_0 f, f \rangle$$

where $H_0 = -\Delta$ with Dirichlet boundary conditions.

Proof. We consider only the standard orthonormal basis of $\mathbf{R}^N$. Applying Lemma 15 to the integration with respect to x_i leads to the formula

$$\int_\Omega \frac{|f(x)|^2}{4d_i(x)^2}\,\mathrm{d}^N x \leqslant \int_\Omega \left|\frac{\partial f}{\partial x_i}\right|^2 \mathrm{d}^N x.$$

The lemma follows by summing over i.

THEOREM 17. *Let the function $m(x)$ be defined on Ω by*

$$\frac{1}{m(x)^2} = \int_{\|u\|=1} \frac{1}{d_u(x)^2}\,\mathrm{d}S(u) \tag{14}$$

where $\mathrm{d}S$ is the standard measure on the unit sphere of $\mathbf{R}^N$, normalised to have total area unity. Then we have $0 \leqslant X \leqslant H_0$, where

$$X(x) = \frac{N}{4m(x)^2}$$

and H_0 is minus the Laplacian with Dirichlet boundary conditions.

Proof. Averaging over all orthonormal bases leads from Lemma 16 to the formula

$$\int_\Omega \frac{N|f(x)|^2}{4m(x)^2}\,\mathrm{d}^N x \leqslant \langle H_0 f, f\rangle$$

for all $f \in C_c^\infty(\Omega)$. The theorem now results from the fact that $C_c^\infty(\Omega)$ is a quadratic form core of H_0.

The evaluation of $X(x)$ in the above theorem is only a matter of computing certain integrals, which may in many cases be directly estimated. The following theorem allows a comparison to be made between $m(x)$ and

$$d(x) = \min\{\|x - y\| : y \notin \Omega\}.$$

Since it is obvious that

$$m(x) \geqslant d(x)$$

for all $x \in \Omega$ and all regions Ω, we seek an estimate in the reverse direction.

We say that the boundary $\partial\Omega$ satisfies a θ-cone condition if every $x \in \partial\Omega$ is the vertex of a circular cone C_x of semi-angle θ which lies entirely within $\mathbf{R}^N \setminus \Omega$ (many similar but weaker conditions can be treated in the same manner). We let $\omega(\alpha)$ denote the solid angle subtended at the origin by a ball of radius $\alpha < 1$ whose centre is at a distance 1 from the origin. Explicitly

$$\omega(\alpha) = \int_0^{\sin^{-1}\alpha} \sin^{n-2}(t)\,\mathrm{d}t \Big/ 2\int_0^{\pi/2} \sin^{n-2}(t)\,\mathrm{d}t.$$

THEOREM 18. *If $\partial\Omega$ satisfies a θ-cone condition then*

$$d(x) \leqslant m(x) \leqslant 2d(x)\,\omega^{-1/2}\left(\frac{\sin\theta}{2}\right)$$

for all $x \in \Omega$.

Proof. Let $x \in \Omega$, $y \in \partial\Omega$ and

$$\|x - y\| = d(x).$$

If u is the unit vector directed along the axis of the exterior cone C_y, then the ball with centre $y + d(x)u$ and radius $d(x)\sin\theta$ lies within C_x and therefore entirely outside U. The solid angle subtended by this ball at x is at least $\omega\left(\frac{1}{2}\sin\theta\right)$ and every line from x within the solid angle meets $\mathbf{R}^N\setminus\Omega$ at a distance at most $2d(x)$ from x. These facts enable one to obtain a lower bound on the integral in (14).

6. LOWER BOUNDS ON THE SMALLEST EIGENVALUE

The whole point of Theorem 17 was that it yields a lower bound on H_0 which varies from point to point, and becomes very large near the boundary of Ω. Nevertheless the theorem easily yields a new lower bound on the smallest eigenvalue of H_0 as follows.

THEOREM 19. *If H_0 is minus the Laplacian on $L^2(\Omega)$ with Dirichlet boundary conditions, where Ω is any open subset of $\mathbf{R}^N$, then*

$$H_0 \geqslant \frac{N}{4\mu^2} \tag{15}$$

where the "quasi-inradius" μ of Ω is defined by

$$\mu = \sup\{m(x) : x \in \Omega\}$$

and $m(x)$ is given by (14).

NOTE. Defining the ordinary inradius δ of Ω by

$$\delta = \sup\{d(x) : x \in \Omega\}$$

we see that δ and μ are of the same order of magnitude in the circumstances of Theorem 18. We emphasise that the bound (15) does not depend upon any topological assumptions on Ω, nor on any regularity property of the boundary $\partial\Omega$. Moreover unlike most other lower bounds on H_0, the one given by (15) decreases monotonically as the region increases. If the boundary is suitably regular then μ may be related to the ordinary inradius by Theorem 18, or one of its many variants.

There are many different lower bounds on H_0 in the literature, for example [6, 7, 8, 9, 14], and almost all are better in some circumstances than any other. This new bound is no exception. If $N \geqslant 2$ and Ω is any region in $\mathbf{R}^N$, then the smallest eigenvalue of H_0 is affected very little by removing from Ω a large finite number of balls, provided those balls have a small enough radius. Similarly the quasi-inradius μ is little affected by such a procedure, although the ordinary inradius may be greatly reduced.

We finally mention that in spite of its crucial importance if $N = 2$ [6, 8, 9], the ordinary inradius is of much less significance if $N \geqslant 3$. For exmple, if Ω is a unit ball in $\mathbf{R}^N$ then the inradius can be reduced as much as one likes by removing line segments from Ω, without affected H_0 or its smallest eigenvalue, because Dirichlet boundary conditions on submanifolds of codimension $\geqslant 2$ have no effect. Thus one cannot get a lower bound on H_0 in terms of the inradius alone, even for contractible regions, if $N \geqslant 3$. On the other hand the bound (15) is useful in all dimensions.

APPENDIX 1

We draw attention to the fact that a result of Glimm and Jaffe [5] was quoted incorrectly in Proposition 15 of [4]. If $H_0 \geqslant 0$ and $V \geqslant 0$ then in order to deduce that

$$\mathrm{Dom}(H_0 \dotplus V) = \mathrm{Dom}(H_0) \cap \mathrm{Dom}\,(V) \tag{16}$$

one needs not

$$0 \leqslant \beta^2 V^2 \leqslant (H_0 \dotplus V)^2 \tag{17}$$

for some $\beta > 0$, but

$$0 \leqslant \alpha^2 H_0^2 + \beta^2 V^2 \leqslant (H_0 \dotplus V)^2 \tag{18}$$

for some $\alpha > 0$ and $\beta > 0$. However this error was not serious in [4] because the quadratic form inequality proved in [4, Lemma 4] could have been written as

$$0 \leqslant H_0^2 + \left(1 - \frac{\alpha}{2}\right) V^2 \leqslant (H_0 \dotplus V)^2.$$

In the present paper we have indeed only proved (17), and so are not justified in claiming (16). This explains the rather unusual care we have taken to obtain all our bounds by limiting procedures from the case of bounded potentials.

Note that in the subsequent paper of Simon [12], only the bound (17) was discussed. In his problem one can deduce (16) from (17) since V is only singular at $x = 0$, and $C_c^\infty(\mathbf{R}^3 \setminus 0)$ is a form core of H_0 on $L^2(\mathbf{R}^3)$.

APPENDIX 2

We have, for the sake of simplicity, assumed throughout the paper that W lies in a certain class $\mathscr{G}$ of functions which are continuously differentiable away from some relatively closed null set S. For the sake of applications it is worth noting that the continuity of the partial derivatives can be replaced by a requirement that the weak (distributional) partial derivatives of W are functions which are locally bounded away from S. In Lemma 1, for example it is sufficient that W be continuous with weak partial derivatives which all lie in $L^\infty(\Omega)$. All the main results of the paper can be modified in an obvious manner, with the occasional necessity of interpreting inequalities as true almost everywhere in $\Omega \setminus S$ instead of everywhere.

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