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Semiclassical Spectral Bounds and Beyond

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1. Setting of the Problem. Lieb-Thirring bounds.

Let

$$H(V) = (-\Delta)^l - V(x), \qquad l > 0, \ x \in \mathbb{R}^d,$$

be a Schrödinger type operator of order 2l on $L^2(\mathbb{R}^d)$. For suitable potential wells $-V(x) \leq 0^1$ the spectrum of H(V) consists of an essential part $\sigma_{ess}(H(V)) = [0, +\infty)$ and of negative eigenvalues $-\lambda_j(V)$. We number these eigenvalues in increasing order counting multiplicities and study the sums

$$S_{d,\gamma}(V) = \sum_{j} \lambda_{j}^{\gamma} = \operatorname{Tr} (H(V))_{-}^{\gamma}, \quad \gamma \geq 0.$$

For $\gamma = 0$ these spectral averages are understood as the counting function for the negative eigenvalues of H(V). The Lieb-Thirring estimates

$$S_{d,\gamma}(V) \le R(d,\gamma,l)S_{d,\gamma}^{\text{cl}}(V) \tag{1}$$

compare the spectral quantities $S_{d,\gamma}(V)$ with the classical phase space averages

$$S^{\mathrm{cl}}_{d,\gamma}(V) = \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^{2l} - V(x))_{-} \frac{dx d\xi}{(2\pi)^d} = L^{\mathrm{cl}}_{d,\gamma,l} \int_{\mathbb{R}^d} V^{\gamma+\varkappa}(x) dx \,,$$

where

$$L_{d,\gamma,l}^{\mathrm{cl}} = \frac{\gamma \Gamma(\gamma) \Gamma(\varkappa + 1)}{2^d \pi^{\frac{d}{2}} \Gamma(\frac{d}{2} + 1) \Gamma(\varkappa + \gamma + 1)} \quad \text{and} \quad \varkappa = \varkappa(d,l) = \frac{d}{2l} \,.$$

Put $\gamma_{\rm CT} = 1 - \varkappa$. The bound (1) holds true for all $V \in L_{\gamma + \varkappa}(\mathbb{R}^d)$, if and only if

$$\gamma \ge \gamma_{\rm cr}$$
 for dimensions $d < 2l$, (2)

$$\gamma > \gamma_{\rm Cr} = 0$$
 for the dimension $d = 2l$, (3)

$$\gamma \ge 0$$
 for dimensions $d > 2l$. (4)

The cases l=1 and $\gamma>0$ for $d\geq 2$ or $\gamma>\frac{1}{2}$ for d=1 respectively, have been settled in the original paper [1]. Their method extends immediately to arbitrary l>0 for all $\gamma>\max\{0,\gamma_{\rm Cr}\}$. The important special case $\gamma=0$ for d>2l has been solved in [2] (for l=1), in [3, 4] (for $l\in\mathbb{N}$) and in [5]. The techniques in the latter paper apply for all l>0. The case $\gamma=\gamma_{\rm Cr}>0$ for d<2l has been proven in [6] for l=1 and in [7] for $l\in\mathbb{N}$. In view of a remark by Simon [8] these methods extend actually to all l>0 [9].

It has also been shown that for $l \in \mathbb{N}$ in the case of d < 2l for $0 < \gamma \le \gamma_{\mathrm{Cr}}$ and for $\gamma = 0$ if d = 2l a reverse bound

$$S_{d,\gamma}(V) \ge \tilde{R}(d,\gamma,l)S_{d,\gamma}^{\text{cl}}(V) \tag{5}$$

holds true for all $0 \leq V \in L_{\gamma+\varkappa}(\mathbb{R}^d)$ with suitable positive constants $\tilde{R}(d,\gamma,l)$, see [10] for $d=l=1, \ \gamma=\gamma_{\rm Cr}$ and [11] for $d=l=1, \ \gamma<\gamma_{\rm Cr}$, as well as [7] for $l\in\mathbb{N}$ and $0<\gamma=\gamma_{\rm Cr}$ and [12] for $l\in\mathbb{N}$ and $0<\gamma<\gamma_{\rm Cr}$. The subtle case $\gamma=\gamma_{\rm Cr}=0$ has been settled in [13]. As a consequence for $l\in\mathbb{N}, \ \gamma=\gamma_{\rm Cr}>0$ and all non-negative $V\in L_1(\mathbb{R}^d)$ one has actually a two-sided bound

$$\tilde{R}(d, \gamma_{\rm cr}) S_{d, \gamma_{\rm cr}}^{\rm cl}(V) \le S_{d, \gamma_{\rm cr}}(V) \le R(d, \gamma_{\rm cr}) S_{d, \gamma_{\rm cr}}^{\rm cl}(V)$$
(6)

with some positive $\tilde{R}(d, \gamma_{\rm cr})$.

For non-integer l>0 and $0\leq\gamma\leq\gamma$ cr the validity of (5) - and hence the validity of the lower bound in (6) - remains open so far.

¹ For simplicity we assume throughout the paper that V(x) > 0 unless explicitly stated otherwise.

2. Sharp Lieb-Thirring constants

We turn now to the optimal values of the constants $R(d, \gamma, l)$ in (1). The discussion of these quantities is governed by two basic facts: Namely, for fixed d and l the functions $R(d, \gamma, l)$ are non-increasing in γ and, moreover, $R(d, \gamma, l) \geq 1$. The first observation is due to Aizenman and Lieb [14], the second one is an immediate consequence of the large coupling asymptotics

$$S_{d,\gamma}(\alpha V) = (1 + o(1))S_{d,\gamma}^{\mathbf{cl}}(\alpha V) \quad \text{as} \quad \alpha \to +\infty.$$
 (7)

Hence, if we have $R(d, \gamma_0, l) = 1$ for some value γ_0 , then for this dimension d it also holds $R(d, \gamma, l) = 1$ for all $\gamma \geq \gamma_0$. Similarly, one has $\tilde{R}(d, \gamma, l) \leq 1$ for all $0 < \gamma \leq \gamma_{\rm Cr}$. Note that the Aizenman-Lieb trick does not work downwards for the lower bounds.

The sharp values of $R(d, \gamma, l)$ are known only in the following two cases

$$R\left(1, \frac{1}{2}, 1\right) = 2$$
 and $R\left(d, \gamma, 1\right) = 1$ for all $\gamma \ge \frac{3}{2}, d \in \mathbb{N}$. (8)

In the first case l=d=1 and $\gamma=\gamma_{\rm Cr}=\frac{1}{2}$ the constant $R\left(1,\frac{1}{2},1\right)=2$ corresponds to the asymptotic behaviour of the weak coupling bound state. Indeed, for smooth and compactly supported $V\geq 0$ one has exactly one negative eigenvalue for all sufficiently small $\alpha>0$ and (see [15])

$$S_{1,\frac{1}{2}}(\alpha V) = (1+o(1))S_{1,\frac{1}{2}}^{\mbox{cl}}(\alpha V) \quad \mbox{as} \quad \alpha \rightarrow +0 \,. \label{eq:S1}$$

By scaling this corresponds to the fact that the constant $R(1, \frac{1}{2}, 1) = 2$ is "achieved" for the Delta potential $V = \delta(x - x_0)$. This case has been settled in [16]. The second case in (8) corresponds to the large coupling Weyl formula (7). This result has been obtained for the one-dimensional case in [1, 14] and for arbitrary dimensions in [17].

In fact, for l = d = 1 and $\gamma = \gamma_{\rm Cr} = \frac{1}{2}$ the Weyl formula is sharp for the lower bound. That means $\tilde{R}\left(1,\frac{1}{2},1\right) = 1$ and the two-sided estimate takes the form

$$S_{1,\frac{1}{2}}^{\text{cl}}(V) \le S_{1,\frac{1}{2}}(V) \le 2S_{1,\frac{1}{2}}^{\text{cl}}(V)$$

for all $0 \leq V \in L_1(\mathbb{R})$.

There are various non-sharp upper and lower bounds on the constants $R(d,\gamma,1)$. In particular, one has $1 < R(d,\gamma,1)$ for all $\gamma < 1$ [18]. Moreover, $R(d,\gamma,1) \le 2$ for $\frac{1}{2} \le \gamma < 1$ [19] and $R(d,\gamma,1) \le 1.814$ for $1 \le \gamma < \frac{3}{2}$ [20, 21] as well as R(2,1,1) > 1 and $R(1,\gamma,1) > 1$ for $\frac{1}{2} \le \gamma < \frac{3}{2}$ [1, 22].

Much less is known on the values of $R(d, \gamma, l)$ for $l \neq 1$. Not only is there no single case where the sharp value has been established, even natural conjectures based on the case l = 1 seem to fail. For example, in the critical case $\gamma = \gamma_{\rm Cr} = \frac{1}{2}$ for d = l = 1 the sharp constant corresponds to the weak coupling behaviour or equivalently the Delta potential. Since for $\gamma = \gamma_{\rm Cr} > 0$ the weak coupling ground state exists and satisfies [7]

$$S_{d,\gamma_{\rm cr}}(\alpha V) = (1 + o(1))\tau(d,l)S_{d,\gamma_{\rm cr}}^{\rm cl}(\alpha V)$$
 as $\alpha \to +0$,

²This Weyl type formula can be verified by standard methods for sufficiently regular potentials. In all cases when (1) holds true, the asymptotic formula extends to all potentials with finite phase space average $S_{d,\gamma}^{\text{cl}}(V)$. Further below we shall also mention some examples of potentials V with finite $S_{d,\gamma}^{\text{cl}}(V)$, where both (1) and (7) fail.

where $\tau(d,l)=\frac{\pi\frac{d}{2l}}{\sin(\pi\frac{d}{2l})}>1$. It seems reasonable to conjecture that $R(d,\gamma_{\rm Cr},l)=\tau(d,l)$. This hypothesis fails. Indeed, in [23] it has been shown, that for $l\in\mathbb{N}$ and non-trivial, sufficiently regular $V\geq 0$ the operator H(V) has exactly $m(d,l)=\binom{l+\left\lfloor\frac{d}{2}\right\rfloor}{d}$ weak coupling states. Since for weak coupling the higher states do all vanish with higher order in the coupling parameter than the ground state, this does not immediately imply a counter example. But on a closer look one can construct even for d=1 and l=2 a two Delta potential for which $S_{1,\frac{3}{4}}(V)>\tau(1,2)S_{1,\frac{3}{4}}^{\rm Cl}(V)$. For that end one starts with a single Delta potential. Since the corresponding ground state of a 4th order operator changes sign, one can add a second Delta function in the nodal point of the ground state to the potential - and therefore a second negative eigenvalue to the operator - not spoiling the first one. A subtle play with the coupling yields the counter example which is essentially based on the presence of two negative eigenvalues [24]. Therefore it seems reasonable to put forward a modified working conjecture that for $\gamma_{\rm Cr}>0$ one has $R(d,\gamma_{\rm Cr},l)=\tau(d,l)$ if and only if m(d,l)=1 and $R(d,\gamma_{\rm Cr},l)>\tau(d,l)$ otherwise.

3. Further Developments

Although the knowledge on sharp constants is now about the same as in the year 2000, the subject sparked quite a substantial amount of work on semiclassical spectral estimates during the past decade. Let me just mention a few important directions, which shall however not be discussed in detail below.

Let me first mention the amazing observation, that for l=1 and $\gamma \geq 2$ the ratio $S_{d,\gamma}(\alpha V)/S_{d,\gamma}^{\rm cl}(\alpha V)$ is monotone increasing in α [25, 26]. Therefore, the proof of the Lieb-Thirring bound and the estimate for the corresponding constant can be pushed into the semiclassical limit. This is the first approach to sharp constants, which is directly applicable to higher dimensions and does not reduce the problem to a one-dimensional setting.

In [20, 21] techniques of mass transport have been applied to claim improved estimates on R(d, 1, 1). Moreover, in [27] a beautiful connection between estimates on R(d, 1, 1) and the so-called loop conjecture have been found.

A third line of work concerns improved Lieb-Thirring estimates with additional Hardy type terms [28, 29, 30].

Finally one should mention Lieb-Thirring estimates on graphs [31] and on metric trees [32, 33].

4. Logarithmic Lieb-Thirring estimates

We turn now to the case d=2l, $l \in \mathbb{N}$ and $\gamma = \gamma_{\rm Cr} = 0$. As mentioned above, in [13] the estimate (5) from below has been established, while the corresponding bound (1) from above fails. To see the latter fact one usually makes the following point: For d=2l the operator $H(\alpha V)$ has for any nontrivial $V \geq 0$ and any $\alpha > 0$ at least one negative bound state and $S_{0,d}(\alpha V) \geq 1$, while at the same time $S_{0,d}^{\rm Cl}(\alpha V) \to 0$ as $\alpha \to +0$. Therefore (1) must fail for $\gamma = \gamma_{\rm Cr} = 0$ as $\alpha \to +0$. This argument, although true of course, shows only a part of the full story. In fact, for $\gamma = \gamma_{\rm Cr} = 0$ the bound (1) may fail even in the large coupling limit. Put l=1, d=2l=2 and for p>1 consider the potentials

$$V_p^{(\infty)}(r) = \frac{\chi_{r > e^2}(r)}{r^2 |\ln r|^2 |\ln |\ln r||^{\frac{1}{p}}} \quad \text{and} \quad V_p^{(0)}(r) = \frac{\chi_{r < e^{-2}}(r)}{r^2 |\ln r|^2 |\ln |\ln r||^{\frac{1}{p}}}, \quad r = |x|.$$

Note that $V_p^{(\infty)}, V_p^{(0)} \in L^1(\mathbb{R}^2)$ and therefore both $S_{0,2}^{\text{cl}}(\alpha V_p^{(\infty)}) \sim \alpha$ and $S_{0,2}^{\text{cl}}(\alpha V_p^{(0)}) \sim \alpha$ for $\alpha \to +\infty$. On the other hand it turns out that we have a non-Weyl high coupling asymptotics

$$S_{0,2}(\alpha V_p^{(\infty)}) \sim \alpha^p$$
 and even $S_{0,2}(\alpha V_p^{(0)} - C) \sim \alpha^p$ as $\alpha \to +\infty$

for any $C \ge 0$, see [34, 35]. Hence, for p > 1 even a modified estimate $S_{0,2}(\alpha V_p^{(0)} - C_1) \le C_2 + C_3 S_{0,2}^{\text{cl}}(\alpha V_p^{(0)})$ fails for arbitrary $C_j > 0$. In search for a replacement of a critical Lieb-Thirring bound for d = 2 and l = 1 one can

In search for a replacement of a critical Lieb-Thirring bound for d=2 and l=1 one can now look on the weak coupling behaviour. Indeed, for sufficiently regular V one has again exactly one weak coupling state $-\lambda_1(\alpha V)$ satisfying

$$\frac{4\pi}{|\ln \lambda_1(\alpha V)|} = (1 + o(1))\alpha \int_{\mathbb{R}^2} V dx = (1 + o(1))CS_{0,2}^{\text{cl}}(\alpha V) \quad \text{as} \quad \alpha \to +0.$$

This motivates to study sums $\sum_{j} F_s(\lambda_j(V))$, where

$$F_s(t) = \frac{1}{|\ln t s^2|}$$
 as $0 < t \le \frac{1}{e s^2}$ and $F_s(t) = 1$ for $0 < \frac{1}{e s^2} < t$.

Note that $F_s(0+) = 0$ and the weak coupling result reads as follows

$$F_s(\varkappa_1(\alpha V)) \sim \frac{\alpha}{4\pi} \int V(x) dx$$
 as $\alpha \to +0$.

This supports the goal to estimate $\sum_j F_s(\lambda_j)$ by a term proportional to $\int V(x)dx$. On the other hand, for large t the function $F_s(t)$ coincides with the counting function and for $V = V_p^{(0)}$ as above we find

$$\sum_{j} F_s(\lambda_j(\alpha V_p^{(0)})) \ge S_{0,2} \left(\alpha V_p^{(0)} - \frac{1}{es^2}\right) \sim \alpha^p \quad \text{as} \quad \alpha \to +\infty.$$

Hence, a straightforward bound of $\sum_{j} F_s(\lambda_j(\alpha V))$ by $\alpha \int V dx = CS_{0,2}^{\text{cl}}(\alpha V)$ is not possible. Our main result is as follows (joint work with H. Kovařík and S. Vugalter [36]):

Theorem 4.1. Put d = 2, l = 1 and $V \ge 0$. Then for any p > 1 and s > 0 it holds

$$\sum_{j} F_s(\lambda_j) \le c_1 \int_{|x| < s} V(x) |\ln |x| s^{-1} |dx + c_p \int_0^{+\infty} r dr \left(\int_0^{2\pi} |V(r, \theta)|^p d\theta \right)^{1/p} ,$$

where the constants c_1 and c_p are independent of s and V. If V is spherical symmetric, then there exists a constant c_0 , such that

$$\sum_{j} F_s(\lambda_j) \le c_1 \int_{|x| < s} V(x) |\ln |x| s^{-1} |dx + c_0| V \|_{L^1(\mathbb{R}^2)}.$$

The r.h.s. of these bounds is homogeneous of degree 1 in V, cf. also [37, 38, 39]. Hence, it reflects the (standard) correct order of the l.h.s. in the weak as well as in the strong coupling limit. Moreover, the finiteness of the r.h.s. fails for potentials $V = V_p^{(0)}$ and excludes non-Weyl asymptotics of deep eigenvalues. On the other hand, the theorem allows for potentials $V = V_p^{(\infty)}$. The non-Weyl asymptotics of the number of negative eigenvalues is compensated by the fact that these eigenvalues stay mainly close to the origin. In fact, the theorem gives estimates on the rate of accumulation of these eigenvalues.

It remains as an open question, whether a similar bound holds true for l = 1/2 in the dimension d = 1, or in general for l = d/2.

5. Setting of the problem: Berezin-Li-Yau inequalities

Let $\Omega \subset \mathbb{R}^d$ be an open domain. We consider $-\Delta_D^{\Omega}$ on $L^2(\Omega)$ with Dirichlet boundary conditions at $\partial\Omega$ defined in the form sense.³ We assume the spectrum of $-\Delta_D^{\Omega}$ to be discrete, e.g. Ω is of finite volume, and denote by

$$0 < \lambda_1(\Omega) \le \lambda_2(\Omega) \le \lambda_3(\Omega) \le \cdots$$

the ordered sequence of the eigenvalues counting multiplicities. Let

$$n(\Omega, \Lambda) := \#\{\lambda_i(\Omega) < \Lambda\}, \quad \Lambda > 0,$$

denote the counting function of this spectrum. Along with the counting function we study the spectral averages

$$S_{d,\gamma}(\Omega,\Lambda) = \sum_{n} (\Lambda - \lambda_n)_+^{\gamma} = \gamma \int_0^{\Lambda} (\Lambda - \tau)^{\gamma - 1} n(\Omega,\tau) d\tau, \quad \Lambda \ge 0, \ \gamma > 0.$$

and

$$s_{d,\gamma}(\Omega,N) = \sum_{k=1}^{N} \lambda_k^{\gamma} = \gamma \int_0^{\infty} \tau^{\gamma-1} (N - n(\Omega,\tau))_+ d\tau, \quad \gamma > 0.$$

In 1912 Weyl proved [40] that for high energies the counting function behaves asymptotically as the corresponding classical phase space volume

$$n(\Omega, \Lambda) = (1 + o(1))n^{cl}(\Omega, \Lambda)$$
 as $\Lambda \to +\infty$,

where

$$n^{cl}(\Omega, \Lambda) = \int_{x \in \Omega} \int_{\xi \in \mathbb{R}^d: |\xi|^2 < \Lambda} \frac{dx \cdot d\xi}{(2\pi)^d} = \frac{\omega_d}{(2\pi)^d} \operatorname{vol}(\Omega) \Lambda^{d/2} = L^{cl}_{d,0} \operatorname{vol}(\Omega) \Lambda^{d/2}.$$

Here ω_d stands for the volume of the unit sphere in \mathbb{R}^d . This formula holds for all domains with finite volume, see also [41]. An integration of this asymptotics gives

$$S_{d,\gamma}(\Omega,\Lambda) = (1+o(1))\gamma \int_0^{\Lambda} (\Lambda-\tau)^{\gamma-1} \frac{\omega_d}{(2\pi)^d} \operatorname{vol}(\Omega)\tau^{d/2} d\tau$$
$$= (1+o(1))S_{d,\gamma}^{cl}(\Omega,\Lambda) \quad \text{as} \quad \Lambda \to +\infty$$

with the corresponding classical phase space average

$$\begin{split} S^{cl}_{d,\gamma}(\Omega,\Lambda) &:= \int_{x\in\Omega} \int_{\xi\in\mathbb{R}^d} (\Lambda-|\xi|^2)_+^{\gamma} \frac{dx\cdot d\xi}{(2\pi)^d} = L^{cl}_{d,\gamma} \mathrm{vol}(\Omega) \Lambda^{\gamma+d/2}\,, \\ L^{cl}_{d,\gamma} &:= \frac{\Gamma(\gamma+1)}{2^d\pi^{d/2}\Gamma(1+\gamma+d/2)} = \gamma B\left(\gamma,1+\frac{d}{2}\right) L^{cl}_{d,0}\,. \end{split}$$

Analogously it holds

$$s_{d,\gamma}(\Omega,\Lambda) = (1+o(1))\gamma \int_0^\infty \tau^{\gamma-1} \left(N - L_{d,0}^{cl} \operatorname{vol}(\Omega)\tau^{d/2}\right)_+ d\tau$$
$$= (1+o(1))s_{d,\gamma}^{cl}(\Omega,N) \quad \text{as} \quad N \to +\infty,$$
$$s_{d,\gamma}^{cl}(\Omega,N) = c(d,\gamma) \left(\operatorname{vol}(\Omega)\right)^{-\frac{2\gamma}{d}} N^{1+\frac{2\gamma}{d}},$$

³From now on we put always l=1 and drop it from the corresponding notation. In particular, $L_{d,\gamma}^{\rm cl}=L_{d,\gamma,1}^{\rm cl}$

with the asymptotical constant

$$c(d,\gamma) := \frac{2\gamma}{d} \left(L_{d,0}^{cl} \right)^{-\frac{2\gamma}{d}} B\left(\frac{2\gamma}{d}, 2 \right) = \frac{d}{2\gamma + d} \left(L_{d,0}^{cl} \right)^{-\frac{2\gamma}{d}} .$$

6. Pólya-Berezin-Lieb-Li-Yau bounds

Again, the semiclassical quantities serve as universal bounds for the corresponding spectral quantities of the Dirichlet Laplacian. In particular, for arbitrary $d \in \mathbb{N}$ and $\gamma \geq 0$ it holds true:

$$n(\Omega, \Lambda) \leq r(d, 0)n^{cl}(\Omega, \Lambda), \quad \Lambda > 0,$$
 (9)

$$S_{d,\gamma}(\Omega,\Lambda) \leq r(d,\gamma)S_{d,\gamma}^{cl}(\Omega,\Lambda), \quad \Lambda > 0,$$
 (10)

$$s_{d,\gamma}(\Omega, N) \geq \rho(d,\gamma) s_{d,\gamma}^{cl}(\Omega, N), \quad N \in \mathbb{N}.$$
 (11)

Here, of course, we have $n(\Omega, \Lambda) = S_{d,0}(\Omega, \Lambda)$ and $n^{cl}(\Omega, \Lambda) = S_{d,0}^{cl}(\Omega, \Lambda)$. In fact, the bounds (9)-(10) can formally be seen as a special case of (1) for potentials $V(x) = \Lambda$ for $x \in \Omega$ and $V(x) = -\infty$ otherwise. In particular, the bound (9) for $d \geq 3$ follows from [5, 3, 4, 2], paper [2] covers also the estimate (9) for d = 2.

But since in this special case the inequalities (9)-(10) hold true for all pairs γ , d with more subtle information on the constants involved, they are usually studied with separate methods. Let us point out the following known information on the constants r and ρ :

$$1 \le r(d,0) \le (1+2d^{-1})^{d/2} \tag{12}$$

$$r(d, \gamma) = 1 \quad \text{for} \quad \gamma \ge 1,$$
 (13)

$$\rho(d, \gamma) = 1 \quad \text{for} \quad \gamma \le 1. \tag{14}$$

The bound (10) with the constant (13) ist due to Berezin [42]. The estimate (11) with (14) has been proven independently by Li any Yau [43]. It also follows from (10) and (13) via Legendre transformation. Both results imply (9) with the upper bound from (12), see also [44].

Pólya proved with a really beautiful argument that r(d,0) = 1 for tiling domains [45] and conjectured that in fact

$$r(d,0) = 1$$
 holds true for arbitrary domains.

Pólya's conjecture remains open so far for general domains, even for the circle! For some generalizations of Pólyas result to product type domains see [44].

7. Pólya's conjecture in the presence of magnetic field

It is an admissible approach in mathematics to learn more abount an interesting but difficult problem by stuying modifications of the original setting. Here we shall include a magnetic field: Let A(x) be a real-valued vector field and consider the magnetic Laplacian

$$(i\nabla + \mathcal{A}(x))^2_{D,\Omega}$$

on $\Omega \subset \mathbb{R}^d$ with Dirichlet boundary conditions at $\partial\Omega$. To distinguish the magnetic case we shall simply enter \mathcal{A} into the notations introduced above.

This modification is motivated by the following observations. Firstly, the inclusion of a magnetic field does not change the phase space volume. Secondly, it is known that if A induces a constant magnetic field, then [46]

$$S_{d,\gamma}(\Omega,\Lambda;\mathcal{A}) \leq S_{d,\gamma}^{cl}(\Omega,\Lambda),$$

for all $\gamma \geq 1$. Moreover, if we restrict ourselves to $\gamma \geq \frac{3}{2}$ then this result extends to arbitrary magnetic fields A (with sufficient regularity to define the magnetic operator in the usual form sense) [17]. In both cases the presence of the magnetic field does not spoil neither the inequality nor the sharp value of the constant therein. Therefore it seems reasonable to ask, whether this behaviour extends to the case $\gamma < 1$ and, in particular, to the case of Pólya's conjecture $\gamma = 0$.

Our main result disproves Pólya's conjecture in the presence of a magnetic field (joint work with R. Frank and M. Loss [47]):

Theorem 7.1. Put d=2 and let $\mathcal{A}=\frac{B}{2}(x_2,-x_1)$ induce a constant magnetic field B. Then there exist constants R_{γ} independent of B, such that

$$S_{2,\gamma}(\Omega, \Lambda, \mathcal{A}) \le R_{\gamma} S_{2,\gamma}^{cl}(\Omega, \Lambda), \quad 0 \le \gamma < 1,$$

where the optimal value of the B-independent constant R_{γ} is given by

$$R_{\gamma} = 2\left(\frac{\gamma}{1+\gamma}\right)^{\gamma} > 1 \quad for \quad 0 \le \gamma < 1.$$

The constant R_{γ} cannot be improved - not even for tiling domains! The example is provided on squares balancing the size of the square with the strength of the magnetic field in a suitable way.

An immediate lesson from this result is that one cannot prove Pólya's original conjecture by methods which extend to the magnetic case. A second lesson is that Pólya's proof is in fact not so much about phase space volume but about the density of states. Indeed, if one allows for *B*-dependent estimates, then for $0 \le \gamma < 1$, $\mathcal{A} = \frac{B}{2}(x_2, -x_1)$ and tiling Ω it holds [47]

$$S_{2,\gamma}(\Omega, \Lambda, \mathcal{A}) \le \mathfrak{B}_{\gamma}(B, \Lambda) \operatorname{vol}(\Omega), \quad \mathfrak{B}_{\gamma}(B, \Lambda) = \frac{B}{2\pi} \sum_{k \ge 0} (\Lambda - B(2k+1))_{+}^{\gamma},$$
 (15)

and the constants $\mathfrak{B}_{\gamma}(B,\Lambda)$ are sharp. For $\gamma=0$ the quantity $\mathfrak{B}_{0}(B,\Lambda)$ is just the density of states of the Landau Hamiltonian!

It remains open, whether an estimate (15) holds true for general domains.

8. Two-term spectral bounds

Weyl conjectured also a two-term asymptotical formula for the counting function

$$n(\Omega, \Lambda) = L_{d,0}^{cl} \operatorname{vol}(\Omega) \Lambda^{d/2} - \frac{1}{4} L_{d-1,0}^{cl} |\partial \Omega| \Lambda^{(d-1)/2} + o(\Lambda^{(d-1)/2}) \quad \text{as} \quad \Lambda \to +\infty.$$

Here the first term on the r.h.s. equals $n^{cl}(\Omega, \Lambda)$. This formula holds true under certain geometrical conditions on the domain [48]. Integrating this asymptotic formula gives

$$\begin{split} S_{d,\gamma}(\Omega,\Lambda) &= L_{d,\gamma}^{cl} \mathrm{vol}(\Omega) \Lambda^{\gamma+d/2} - \frac{1}{4} L_{d-1,\gamma}^{cl} |\partial \Omega| \Lambda^{\gamma+(d-1)/2} + o(\Lambda^{\gamma+(d-1)/2}), \\ s_{d,\gamma}(\Omega,N) &= c(d,\gamma) \left(\mathrm{vol}(\Omega) \right)^{-\frac{2\gamma}{d}} N^{1+\frac{2\gamma}{d}} \\ &+ \frac{L_{d-1,\gamma}^{cl} \left(L_{d,\gamma}^{cl} \right)^{-1-\frac{2\gamma-1}{d}}}{4(\frac{d-1}{2} + \gamma)} \cdot \frac{\gamma |\partial \Omega|}{\left(\mathrm{vol}(\Omega) \right)^{1+\frac{2\gamma-1}{d}}} N^{1+\frac{2\gamma-1}{d}} + o(N^{1+\frac{2\gamma-1}{d}}). \end{split}$$

Again, the first terms on the r.h.s. equal $S_{d,\gamma}^{cl}(\Omega,\Lambda)$ and $s_{d,\gamma}^{cl}(\Omega,N)$, respectively. At least for $\gamma \geq 1$ the geometrical conditions on the domain Ω can largely be dropped [49].

Note that the signs of the lower order terms seem to suggest, that the spectral bounds (10)-(11) with sharp first order Weyl term (13)-(14) could possibly be improved by additional terms reflecting the second order corrections.

Trying to prove such bounds one should first note that any bound

$$S_{d,\gamma}(\Omega,\Lambda) \leq S_{d,\gamma}^{cl}(\Omega,\Lambda) - C \cdot |\partial \Omega| \Lambda^{\gamma + \frac{d-1}{2}}$$

must fail in general. Indeed, adding "needles" to a domain Ω one can increase the perimeter $|\partial\Omega|$ arbitrarily without changing the volume of Ω a lot, and the r.h.s. of this bound would turn even negative. Therefore, part of the problem is to replace $|\partial\Omega|$ by some other suitable geometric value.

9. Melas' bound

A first step towards this direction was made by Melas [50]. Let for an open domain $\Omega \subset \mathbb{R}^d$

$$J(\Omega) = \min_{y \in \mathbb{R}^d} \int_{\Omega} |x - y|^2 dx$$

be its moment. Then the following bound holds true

$$s_{d,1}(\Omega, N) \ge c(d, 1) \left(\operatorname{vol}(\Omega)\right)^{-\frac{2}{d}} N^{1+\frac{2}{d}} + M(d) \frac{\operatorname{vol}(\Omega)}{J(\Omega)} N. \tag{16}$$

Via Legendre transformation this turns into [51]

$$S_{d,1}(\Omega, \Lambda) \le S_{d,1}^{cl} \left(\Omega, \Lambda - M_d \frac{\operatorname{vol}(\Omega)}{J(\Omega)}\right).$$
 (17)

This bound is remarkable, since it works at the endpoint $\gamma = 1$ of the scale, where the Li-Yau and the Berezin bounds are proven with sharp semiclassical constants. On the other hand, the correction term of order O(N) is not of the expected order $O(N^{1+\frac{1}{d}})$. The same holds in the Berezin picture (17).

10. Improved Berezin bounds with remainder terms of correct order

Consider an open domain $\Omega \subset \mathbb{R}^d$. Choose a coordinate system in \mathbb{R}^d and put $\mathbb{R}^d \ni x = (x', x_d) \in \mathbb{R}^{d-1} \times \mathbb{R}$. For fixed $x' \in \mathbb{R}^{d-1}$ the intersection of $\{(x', t), t \in \mathbb{R}\} \cap \Omega$ consists of

at most countable many intervals. Let $\Omega_{\Lambda}(x')$ be the union of all such intervals, which are longer than $l_{\Lambda} := \pi \Lambda^{-1/2}$. The number of these intervals is denoted by $\varkappa(x', \Lambda)$. Put

$$\Omega_{\Lambda} = \bigcup_{x' \in \mathbb{R}^{d-1}} \Omega_{\Lambda}(x') \subset \Omega \quad \text{and} \quad d_{\Lambda}(\Omega) = \int_{x' \in \mathbb{R}^{d-1}} \varkappa(x', \Lambda) dx'.$$

That means Ω_{Λ} is the subset of Ω , where the intervals of Ω in x_d -direction are longer than l_{Λ} . The set Ω_{Λ} is increasing in Λ . The value $d_{\Lambda}(\Omega)$ is an effective measure of the projection of Ω_{Λ} on the x'-plane counting the number of sufficiently long intervals. It also increases in Λ . Since $\text{vol}(\Omega_{\Lambda}) \geq l_{\Lambda} d_{\Lambda}(\Omega)$, the finiteness of $\text{vol}(\Omega_{\Lambda})$ implies finiteness of $d_{\Lambda}(\Omega)$. It holds [52]

Theorem 10.1. Assume that for a given $\Lambda > 0$ we have $vol(\Omega_{\Lambda}) < \infty$. Then for any $\gamma \geq \frac{3}{2}$

$$S_{d,\gamma}(\Omega,\Lambda) \le L_{d,\gamma}^{cl} vol(\Omega_{\Lambda}) \Lambda^{\sigma + \frac{d}{2}} - \nu(d,\gamma) 4^{-1} L_{d-1,\gamma}^{cl} d_{\Lambda}(\Omega) \Lambda^{\sigma + \frac{d-1}{2}}. \tag{18}$$

The first term on the r.h.s. coincides with $S^{cl}_{d,\gamma}(\Omega_{\Lambda};\Lambda)$, while the correction term is of the expected second Weyl order $O(\Lambda^{\sigma+\frac{d-1}{2}})$. But even the first term is already an improvement over the standard Berezin bound for $\gamma \geq \frac{3}{2}$. Indeed, instead of $\operatorname{vol}(\Omega)$ only the quantity $\operatorname{vol}(\Omega_{\Lambda})$ appears: The bound counts only the volume of the part of the domain, where it is wide enough for sufficiently deep bound states to settle. In particular, one can apply (18) even for domains Ω of infinite volume as long as $\operatorname{vol}(\Omega_{\Lambda})$ is finite. Moreover, the bound (18) extends to the case of arbitrary magnetic fields. However, the techniques applied (sharp Lieb-Thirring inequalities with operator-valued potentials) restrict ourselfs to the case $\gamma \geq \frac{3}{2}$. It would be of great interest to extend this type of results, both regarding the effective reduction of the domain to Ω_{Λ} as well as the appearance of a second order term, to the case $\gamma = 1$.

One can also supply explicite estimates on the constants $\nu(d,\gamma)$. Namely, we have

$$0 < 4\varepsilon \left(\gamma + \frac{d-1}{2}\right) \le \nu(d,\gamma) \le 2$$
,

where

$$\varepsilon(\sigma) = \inf_{a \ge 1} \left(\frac{a}{2} B \left(\sigma + 1, \frac{1}{2} \right) - \sum_{k \ge 1} \left(1 - \frac{k^2}{a^2} \right)_+^{\sigma} \right) .$$

In particular, it holds [54] $\varepsilon(\sigma) = \frac{1}{2}B\left(\sigma+1,\frac{1}{2}\right)$ for $\sigma \geq 3$, and a numerical evaluation gives for the special case d=2 and $\gamma=\frac{3}{2}$

$$1.91 < \nu\left(2, \frac{3}{2}\right) \le 2$$
.

For further applications of (18) to bounds for the heat kernel of the Dirichlet Laplacian see [54].

11. A MORE GEOMETRIC SECOND TERM

The bound (18) as stated above is of particular use, if the domain streches along one distinguished direction, like horn shaped domains, see [54]. Otherwise one would wish for a more intrinsic geometrical second term, which is independent of the choice of the coordinate system. Of course, one can average (18) over all directions, but this does not necessarily yield a more appealing bound.

⁴Such an estimate has been obtained for the discrete Laplacian in [53].

Alternatively, one can "hide" the correction first in a Hardy type term and average afterwards. Indeed, for any $u \in \mathbb{S}^{d-1}$ and $\gamma \geq 3/2$ one can prove (joint work with L. Geisinger and A. Laptev [55]) that

$$S_{d,\gamma}(\Omega,\Lambda) \leq L_{d,\gamma}^{cl} \int_{\Omega} \left(\Lambda - \frac{1}{4 d(x,u)^2}\right)_+^{\gamma + \frac{d}{2}} dx,$$

where

$$\theta(x,u) = \inf\{t > 0 : x + tu \notin \Omega\} \quad \text{and} \quad d(x,u) = \inf\{\theta(x,u), \theta(x,-u)\}.$$

Averaging over the directions gives now rise to the following result. For $x \in \Omega$ let

$$\Omega(x) = \{ y \in \Omega : x + t(y - x) \in \Omega, \ \forall t \in [0, 1] \}$$

be the part of Ω that "can be seen" from x and let $\delta(x) = \inf \{ |y - x| : y \notin \overline{\Omega(x)} \}$ denote the distance to the exterior of $\Omega(x)$. For fixed $\varepsilon > 0$ put

$$A_{\varepsilon}(x) = \left\{ a \in \mathbb{R}^d \setminus \overline{\Omega(x)} : |x - a| < \delta(x) + \varepsilon \right\}$$

and for $a \in A_{\varepsilon}(x)$ set $B_x(a) = \{ y \in \mathbb{R}^d : |y - a| < |x - a| \}$ and

$$\rho_a(x) = \frac{|B_x(a) \setminus \overline{\Omega(x)}|}{\omega_d |x - a|^d},$$

where ω_d denotes the volume of the unit ball in \mathbb{R}^d . Moreover, we put

$$\rho(x) = \inf_{\varepsilon > 0} \sup_{a \in A_{\varepsilon}(x)} \rho_a(x) \quad \text{and} \quad M_{\Omega}(\Lambda) = \int_{R_{\Omega}(\Lambda)} \rho(x) \, dx \,,$$

where $R_{\Omega}(\Lambda) \subset \Omega$ denotes the set $\{x \in \Omega : \delta(x) < 1/(4\sqrt{\Lambda})\}$. The function $\rho(x)$ depends on the behaviour of the boundary close to $x \in \Omega$. For example, $\rho(x)$ is small close to a cusp. On the other hand $\rho(x)$ is larger than 1/2 in a strictly convex domain. By definition, the function $M_{\Omega}(\Lambda)$ gives an average of this behaviour over $R_{\Omega}(\Lambda)$, which is like a tube of width $1/(4\sqrt{\Lambda})$ around the boundary. Its decay for $\lambda \to \infty$ is related to the Minkowski dimension of the boundary.

The following result allows a geometric interpretation of the remainder term (joint work with L. Geisinger and A. Laptev [55]):

Theorem 11.1. Let $\Omega \subset \mathbb{R}^d$ be an open set with finite volume and $\gamma \geq 3/2$. Then

$$S_{d,\gamma}(\Omega,\Lambda) \le L_{d,\gamma}^{cl} \operatorname{vol}(\Omega) \Lambda^{\frac{d}{2}+\gamma} - L_{d,\gamma}^{cl} 2^{-d+1} \Lambda^{\frac{d}{2}+\gamma} M_{\Omega}(\Lambda) \quad \text{for all} \quad \Lambda > 0.$$
 (19)

12. Improving Melas' bound

As stated above, it is of interest to transfer Berezin-Li-Yau bounds with remainder terms of sharp order to the limit case $\gamma=1$ when the first term with sharp constant is known. To understand the difficulties let us have a look on the idea behind the proof of the Li-Yau and Melas inequalities.

Let ψ_j be the o.n. eigenfunctions of $-\Delta_{\Omega}^D$. Put $\hat{\psi}_j(\xi) = (2\pi)^{-d/2}(\psi_j, e^{i\xi x})_{L^2(\Omega)}$ and $F(\xi) = \sum_{j=1}^N |\hat{\psi}_j(\xi)|^2 \ge 0$. Then

$$s_{d,1}(\Omega, N) = \int_{\mathbb{R}^d} |\xi|^2 F(\xi) d\xi = I(F)$$
 (20)

$$N = \int F(\xi)d\xi, \tag{21}$$

$$F(\xi) = \sum_{j=1}^{N} |\hat{\psi}_{j}(\xi)|^{2} \le (2\pi)^{-d} \|e^{i\xi x}\|_{L^{2}(\Omega)}^{2} = (2\pi)^{-d} \operatorname{vol}(\Omega).$$
 (22)

An estimate on $s_{d,1}(\Omega, N) = \sum_{j=1}^{N} \lambda_j$ from below can be obtained minimizing I(F) in (20) for $F \geq 0$ satisfying (21) and (22). A minimizer should be spherical symmetric and non-increasing in the radius and a straightforward application of the bathtub principle leads to the Li-Yau bound with $\rho(d,1) = 1$. Using the momentum of the domain Melas puts forward the additional information $|\nabla F| \leq 2(2\pi)^{-d} \sqrt{J(\Omega)} \operatorname{vol}(\Omega)$. Solving the modified optimization problem leads to his improvement of the bound (16). A quite similar approach has recently been applied in [56, 57] for the Stokes and the Klein-Gordon operator.

But this idea will not yield remainder terms of sharp order. In fact, the true second Weyl term is hidden in Bessel's inequality (22). To quantify it, one has to show that lower Dirichlet eigenfunctions cannot approximate a free wave on the domain too well, since these eigenfunctions must vanish at the boundary. For this one needs to deduce subtle pointwise estimates on Dirichlet eigenfunctions from integral energy estimates. In contrast to the discrete case [53] this proves to be quite difficult in the continuous case. We can provide the following result (joint work with H. Kovařík and S. Vugalter [58]):

Theorem 12.1. Let $\Omega \subset \mathbb{R}^2$ be a polygon with n sides. Let l_j be the length of the j-th side p_j of Ω and let d_j be the distance of the middle third of p_j to $\partial \Omega \setminus p_j$. Then for any $k \in \mathbb{N}$ and any $\alpha \in [0,1]$ we have

$$s_{2,1}(\Omega, N) \geq s_{2,1}^{cl}(\Omega, N) + \frac{4\alpha c_3}{vol(\Omega)^{\frac{3}{2}}} N^{\frac{3}{2} - \epsilon(N)} \sum_{j=1}^{n} l_j \Theta\left(N - \frac{9vol(\Omega)}{2\pi d_j^2}\right) + (1 - \alpha) M(2) \frac{vol(\Omega)}{J(\Omega)} N,$$

where

$$\epsilon(N) = \frac{2}{\sqrt{\log_2(2\pi N/c_1)}}, \qquad c_1 = \sqrt{\frac{3\pi}{14}} \ 10^{-11}, \qquad c_3 = \frac{2^{-3}}{9\sqrt{2} \ 36} (2\pi)^{\frac{5}{4}} c_1^{1/4}.$$

Minimizing the r.h.s. in $\alpha \in [0, 1]$ this is an actual improvement on Melas' bound which corresponds to the case $\alpha = 0$. The second term on the r.h.s. is almost of the expected Weyl order. The result can be extended to non-polygons as well; for details see [58].

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