Improved Berezin-Li-Yau bounds with remainder terms

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0. The Dirichlet Laplacian

Let $\Omega \subset \mathbb{R}^d$ be an open domain. We consider $-\Delta_D^\Omega$ with Dirichlet boundary conditions on $L^2(\Omega)$.

We assume the spectrum of $-\Delta_D^\Omega$ to be discrete (e.g. Ω is bounded or of finite volume) and denote by

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

the ordered sequence of the eigenvalues (counting multiplicities).

Let

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

denote the counting function of the spectrum.

1. Riesz means.

Along with the counting function we study the average spectral quantities

$$S_{\sigma,d}(\Omega,\Lambda) := \sum_n (\Lambda-\lambda_n)_+^\sigma = \sigma\int_0^\Lambda (\Lambda-\tau)^{\sigma-1} n(\Omega,\tau)\,d\tau\,,\quad \Lambda\geq 0,\ \sigma>0.$$

and

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

2. Weyl's Law. The first term.

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

$$n(\Omega,\Lambda) = (1+o(1))\eta(\Omega,\Lambda) \quad \text{as} \quad \Lambda \to +\infty,$$

where

$$\begin{aligned}\eta(\Omega,\Lambda) \quad &:= \quad \int_{x\in\Omega}\int_{\xi\in\mathbb{R}^d:|\xi|^2<\Lambda} \frac{dx\cdot d\xi}{(2\pi)^d} \\ &= \quad \frac{\omega_d}{(2\pi)^d}\mathrm{vol}(\Omega)\Lambda^{d/2} = L_{0,d}^{cl}\mathrm{vol}(\Omega)\Lambda^{d/2}.\end{aligned}$$

This formula holds for all domains with finite volume.

Integration of this formula gives

$$S_{\sigma,d}(\Omega,\Lambda) = (1+o(1))\sigma \int_0^\Lambda (\Lambda-\tau)^{\sigma-1} \underbrace{\frac{\omega_d}{(2\pi)^d}\mathsf{vol}(\Omega)\tau^{d/2}}_{\eta(\Omega,\tau)} d\tau$$

$$= (1+o(1)) S^{cl}_{\sigma,d}(\Omega,\Lambda) \quad \text{as} \quad \Lambda \to +\infty$$

with the corresponding classical phase space average

$$S^{cl}_{\sigma,d}(\Omega,\Lambda) := \int_{x\in\Omega}\int_{\xi\in\mathbb{R}^d} (\Lambda-|\xi|^2)_+^\sigma \frac{dx\cdot d\xi}{(2\pi)^d} = L^{cl}_{\sigma,d}\mathsf{vol}(\Omega)\Lambda^{\sigma+d/2},$$

$$L^{cl}_{\sigma,d} := \frac{\Gamma(\sigma+1)}{2^d\pi^{d/2}\Gamma(1+\sigma+d/2)} = \sigma B\left(\sigma, 1+\frac{d}{2}\right) L^{cl}_{0,d}.$$

Analogously it holds

$$
\begin{aligned}
s_{\sigma,d}(\Omega,\Lambda) &= (1+o(1))\sigma \int_0^\infty \tau^{\sigma-1} \Bigg(N - \underbrace{L^{cl}_{0,d}\mathsf{vol}(\Omega)\tau^{d/2}}_{\eta(\Omega,\tau)} \Bigg)_+ d\tau \\
&= (1+o(1)) s^{cl}_{\sigma,d}(\Omega,N) \quad \text{as} \quad N \to +\infty\,, \\
s^{cl}_{\sigma,d}(\Omega,N) &= c(\sigma,d)\,(\mathsf{vol}(\Omega))^{-\frac{2\sigma}{d}} N^{1+\frac{2\sigma}{d}}\,,
\end{aligned}
$$

with the asymptotical constant

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

3. Polya-Berezin-Lieb-Li-Yau bounds

The semiclassical quantities serve as universal bounds for the corresponding spectral quantities of the Dirichlet Laplacian. In particular, it holds true:

$$\begin{aligned} \#\{\lambda_k < \Lambda\} = n(\Omega,\Lambda) &\leq r(0,d)\eta(\Omega,\Lambda)\,, \quad \Lambda > 0\,, \\ \sum_k (\Lambda - \lambda_k)_+^\sigma = S_{\sigma,d}(\Omega,\Lambda) &\leq r(\sigma,d) S^{cl}_{\sigma,d}(\Omega,\Lambda)\,, \quad \Lambda > 0\,, \\ \sum_{k=1}^N \lambda_k^\sigma = s_{\sigma,d}(\Omega,N) &\geq \rho(\sigma,d) s^{cl}_{\sigma,d}(\Omega,N)\,, \quad N \in \mathbb{N}\,. \end{aligned}$$

Let us point out the following known information on the constants r and ρ:

$$1 \leq r(0,d) \leq (1+2d^{-1})^{d/2} \quad \text{and} \quad 1 = r(0,d) \quad \text{for tiling domains}$$

$$1 = r(\sigma,d) \quad \text{for} \quad \sigma \geq 1 \quad \text{and} \quad 1 = \rho(\sigma,d) \quad \text{for} \quad \sigma \leq 1.$$

4. Weyl's Law. The first term and the second term.

Weyl conjectured also a two-term asymptotical formula for the counting function including the effect of the boundary

$$n(\Omega, \Lambda) = \underbrace{L^{cl}_{0,d}\mathrm{vol}(\Omega)\Lambda^{d/2}}_{\eta(\Omega,\Lambda)} - \frac{1}{4}L^{cl}_{0,d-1}|\partial\Omega|\Lambda^{(d-1)/2} + o(\Lambda^{(d-1)/2})$$

as $\Lambda \to +\infty$.

This formula holds under certain geometrical conditions on the domain (Ivrii).

Integration of this formula gives for $\Lambda \to +\infty$ respectively $N \to +\infty$

$$S_{\sigma,d}(\Omega,\Lambda) = \underbrace{L^{cl}_{\sigma,d}\mathsf{vol}(\Omega)\Lambda^{\sigma+d/2}}_{S^{cl}_{\sigma,d}(\Omega,\Lambda)} - \frac{1}{4}L^{cl}_{\sigma,d-1}|\partial\Omega|\Lambda^{\sigma+(d-1)/2} + o(\Lambda^{\sigma+(d-1)/2}),$$

$$s_{\sigma,d}(\Omega,N) = \underbrace{c(\sigma,d)\,(\mathsf{vol}(\Omega))^{-\frac{2\sigma}{d}}\,N^{1+\frac{2\sigma}{d}}}_{s^{cl}_{\sigma,d}(\Omega,N)}$$

$$+ \frac{L^{cl}_{\sigma,d-1}(L^{cl}_{\sigma,d})^{-1-\frac{2\sigma-1}{d}}}{4(\frac{d-1}{2}+\sigma)} \cdot \frac{\sigma|\partial\Omega|}{(\mathsf{vol}(\Omega))^{1+\frac{2\sigma-1}{d}}} N^{1+\frac{2\sigma-1}{d}} + o(N^{1+\frac{2\sigma-1}{d}})$$

Statement of the Problem: Can on find universal bounds on the spectral quantities containing the sharp first Weyl term *and* reflecting the contribution of the second order term?

$$S_{\sigma,d}(\Omega,\Lambda) \le S^{cl}_{\sigma,d}(\Omega,\Lambda) - C\cdot|\partial\Omega|\Lambda^{\sigma+\frac{d-1}{2}} \quad \text{must fail!}$$

5. The Melas bound

For any open domain $\Omega \subset \mathbb{R}^d$ it holds

$$\sum_{k=1}^{N} \lambda_k = s_{1,d}(\Omega, N) \geq \underbrace{c(1,d)\,(\mathrm{vol}(\Omega))^{-\frac{2}{d}}\, N^{1+\frac{2}{d}}}_{s_{1,d}^{cl}(\Omega,N)} + M(d)\frac{\mathrm{vol}(\Omega)}{J(\Omega)} N$$

where

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

is the momentum of Ω and $M(d)$ depends only on d.

Good: It works for $\sigma = 1$.

Bad: It does not reflect the asymptotical order $O(N^{1+\frac{1}{d}})$ of the correction term.

6. Statement of the result

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 (finite) 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

$$\Omega_\Lambda := \bigcup_{x' \in \mathbb{R}^{d-1}} \Omega_\Lambda(x') \subset \Omega$$

$$d_\Lambda(\Omega) := \int_{x' \in \mathbb{R}^{d-1}} \varkappa(x', \Lambda) dx'$$

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 increases in Λ.

For any open domain $\Omega \subset \mathbb{R}^d$, $\sigma \geq 3/2$ and any $\Lambda > 0$ it holds

$$\sum_k (\Lambda - \lambda_k)_+^\sigma = S_{\sigma,d}(\Omega,\Lambda) \leq \underbrace{L_{\sigma,d}^{cl} \text{vol}(\Omega_\Lambda)\Lambda^{\sigma+\frac{d}{2}}}_{S_{\sigma,d}^{cl}(\Omega_\Lambda;\Lambda)} - \nu(\sigma,d)\frac{1}{4} L_{\sigma,d-1}^{cl} d_\Lambda(\Omega)\Lambda^{\sigma+\frac{d-1}{2}}$$

Good:

- It reflects the correct asymptotical order $O(\Lambda^{\sigma+\frac{d-1}{2}})$ of the correction term.
- The bound feels some geometry via the construction of Ω_Λ and d_Λ: It counts the volume only where the domain is sufficiently wide for a bound state to settle.
- It works for Ω of infinite volume as long as $\text{vol}(\Omega_\Lambda)$ is finite.

Bad:

- It works only for $\sigma \geq 3/2$.

For the constant we have

$$\nu\left(\sigma + \frac{d-2}{2}, 2\right) \le \nu(\sigma, d) \le 2 \quad \text{and} \quad \nu(\sigma, 2) \ge 4\varepsilon(\sigma + 1/2)$$

where $\varepsilon(\sigma + 1/2)$ is the optimal constant for

$$\sum_k (A^2 - k^2)_+^{\sigma+1/2} \le \frac{1}{2} B(\sigma + 3/2, 1/2) A^{2\sigma+2} - \varepsilon(\sigma + 1/2) A^{2\sigma+1}, \quad A \ge 1,$$

to be true. In particular (including a numerical evaluation)

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

7. The key ingredient 1: Sharp Lieb-Thirring bounds for operator valued potentials

Let G be an auxiliary Hilbert space. Consider an function $W : \mathbb{R}^m \to B(G)$ taking values in the set of self-adjoint bounded (compact) operators on G.

We study the Schrödinger type operator

$$H = -\Delta \otimes \mathbf{1}_G - W(x) \quad \text{on} \quad L^2(\mathbb{R}^m, G).$$

Then it holds (Laptev,W.):

$$\mathrm{tr}_{L^2(\mathbb{R}^m,G)}\, H_-^\sigma \leq L_{\sigma,m}^{cl} \int \mathrm{tr}_G W_+^{\sigma+\frac{m}{2}}(x)dx, \quad \sigma \geq 3/2\,.$$

8. The key ingredient 2: Induction in the dimension

We settle as an example the case of $-\Delta_D^\Omega$ for $d = 2$ and $\sigma = 3/2$. A simple variational argument implies

$$-\Delta_D^\Omega - \Lambda = -\frac{\partial^2}{\partial x^2} + \left(-\frac{\partial^2}{\partial y^2} - \Lambda\right) \geq -\frac{d^2}{dx^2} - W_-(x) \text{ on } L_2(\mathbb{R}, L_2(\mathbb{R}))$$

where $W(x) = \left(-\frac{d^2}{dy^2}\right)_D^{\Omega(x)} - \Lambda$ is the shifted second derivative in y-direction on the section $\Omega(x)$ with Dirichlet boundary conditions.

Assume for simplicity first, that this section consists of one interval of length $l(x)$.

Then the k-th eigenvalue of $W(x)$ is given by the identity

$$\mu_k(x) = \pi^2 k^2 l^{-2}(x) - \Lambda, \quad k \in \mathbb{N}.$$

The Lieb-Thirring inequality for operator valued potentials implies now

$$
\begin{aligned}
S_{3/2,2}(\Omega,\Lambda) &\leq \operatorname{tr}\left(-\frac{d^2}{dx^2} - W_-(x)\right)_-^{3/2} \\
&\leq \frac{3}{16}\int_{\mathbb{R}} \operatorname{tr} W_-^2(x)dx \leq \frac{3}{16}\int_{\mathbb{R}} \sum_k (\Lambda - \pi^2 k^2 l^{-2}(x))_+^2 dx \\
&\leq \frac{3}{16}\int_{\mathbb{R}} \frac{\pi^4}{l^4(x)} \sum_{k=1}^{[A(x)]} (A^2(x) - k^2)^2 dx, \quad A(x) = \frac{l(x)}{l_\Lambda}.
\end{aligned}
$$

The integrand in non-zero only where $A(x) > 1$ or equivalently $l(x) > l_\Lambda$.

We denote the set of such x by I_Λ and integration in the formula above takes place over the set I_Λ only.

Let us estimate the sum in the integrand for $A > 1$.

For $A > 1$ it holds

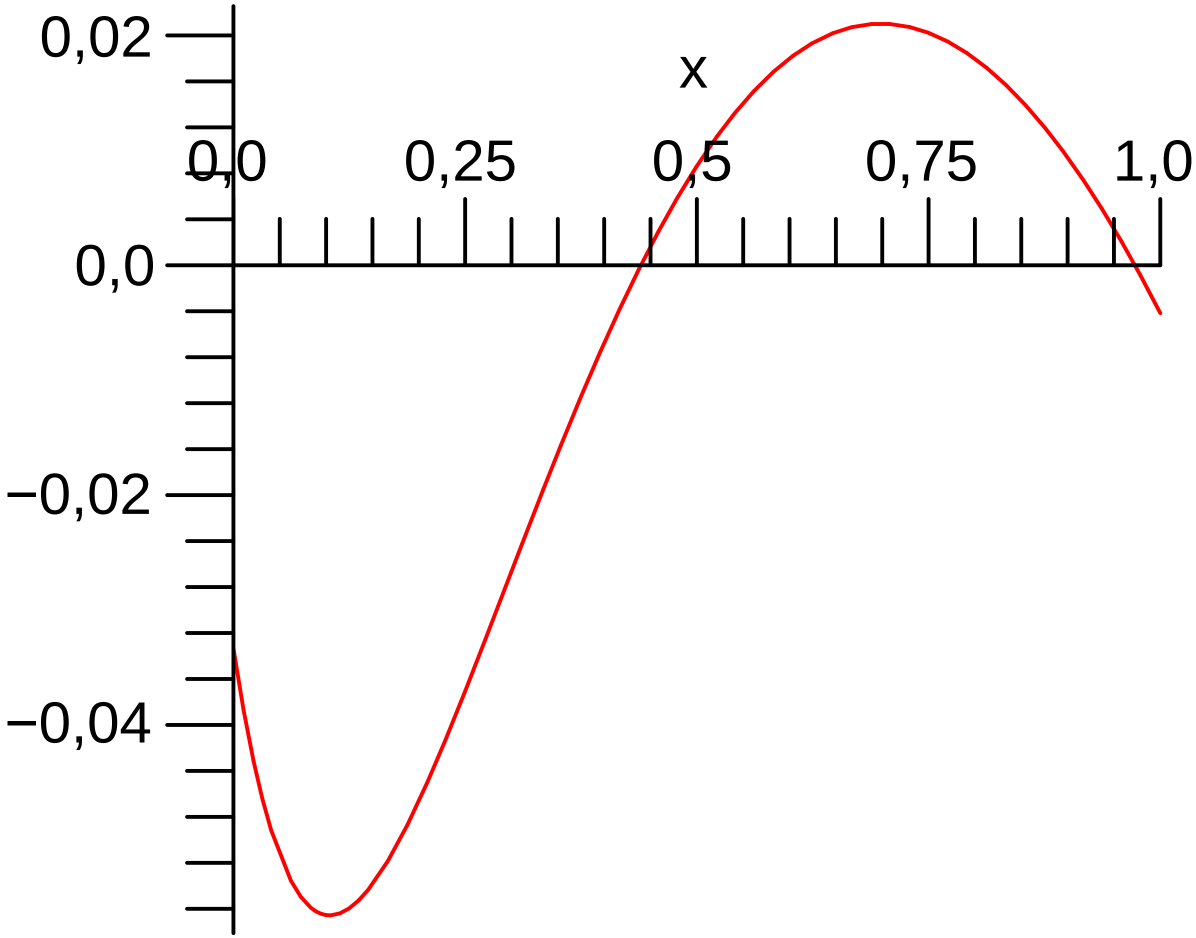
$$\sum_{k=1}^{[A]} (A^2 - k^2)^2 dx \leq \frac{8}{15} A^5 - \left(\frac{1}{2} - \delta \right) A^4 .$$

where δ is the maximum of the function

$$\frac{29}{30} - \frac{2}{(1+x)^2} + \frac{1}{(1+x)^4} - \frac{8x}{15} \quad \text{on} \quad x \in [0,1].$$

A numerical evaluation of δ gives

$$\delta \approx 0.0210228223$$


0,02
x
0,0
0,25
0,5
0,75
1,0
0,0
−0,02
−0,04

9. Improved Berezin-Li-Yau bounds for $\sigma = 3/2$ and $d = 2$

This gives finally with $l = l(x)$ and $A = A(x) = l(x) l_\Lambda^{-1} = \pi^{-1} l(x) \Lambda^{1/2}$

$$\begin{aligned} S_{3/2,2}(\Omega, \Lambda) &\leq \frac{3}{16} \int_{I_\Lambda} \frac{\pi^4}{l^4} \left(\frac{8}{15} \left(\frac{l \Lambda^{1/2}}{\pi} \right)^5 - \left(\frac{1}{2} - \delta \right) \left(\frac{l \Lambda^{1/2}}{\pi} \right)^4 \right) dx \\ &= \frac{3}{16} \cdot \frac{8}{15} \cdot \frac{1}{\pi} \cdot \Lambda^{5/2} \int_{I_\Lambda} l(x) dx - \frac{3}{16} \left(\frac{1}{2} - \delta \right) \Lambda^2 \int_{I_\Lambda} dx \\ &= L^{cl}_{3/2,2} \mathrm{vol}(\Omega_\Lambda) \Lambda^{5/2} - (2 - 4\delta) \cdot \frac{1}{4} \cdot L^{cl}_{3/2,1} \cdot d_\Lambda \Lambda^2 \end{aligned}$$

with $\nu(3/2, 2) = (2 - 4\delta) \approx 1.915908710$. We use that

$$L^{cl}_{3/2,2} = (10\pi)^{-1}, \quad L^{cl}_{3/2,1} = 3/16.$$

10. Berezin-Li-Yau bounds for magnetic fields

Consider the magnetic Laplacian $(i\nabla + \mathcal{A}(x))^2$ with Dirichlet boundary conditions on $\Omega \subset \mathbb{R}^d$. Magnetic fields do not change the phase space volume.

So far there is only one result concerning sharp constants for magnetic fields:

$$S_{\sigma,d}(\Omega, \Lambda, \mathcal{A}) \leq S^{cl}_{\sigma,d}(\Omega_\Lambda), \quad \sigma \geq 1, \quad \text{(Loss, Erdös, Wugalter)}$$

if $\mathcal{A}$ induces a *constant* magnetic field.

Our bound with remainder terms extends to *arbitrary* magnetic fields for $\sigma \geq 3/2$.

11. Open Problems

- Does the Berezin-Li-Yau bound hold for $\sigma = 1$ for arbitrary magnetic fields?

- Does the Polya conjecture hold for constant (arbitrary) magnetic fields even for tiling domains?

- Is there a Melas type bound with a remainder term of correct order?