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. $\Omega$ 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

\[
S_{\sigma,d}(\Omega, \Lambda) := \sum_n (\Lambda - \lambda_n)^{\sigma}_+
\]

\[
= \sigma \int_0^\Lambda (\Lambda - \tau)^{\sigma - 1} n(\Omega, \tau) d\tau, \quad \Lambda \geq 0, \quad \sigma > 0.
\]

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

\[ \eta(\Omega, \Lambda) := \int_{x \in \Omega} \int_{\xi \in \mathbb{R}^d : |\xi|^2 < \Lambda} \frac{dx \cdot d\xi}{(2\pi)^d} \]

\[ = \frac{\omega_d}{(2\pi)^d} \text{vol}(\Omega) \Lambda^{d/2} = I_{0,d}^{cl} \text{vol}(\Omega) \Lambda^{d/2}. \]

This formula holds for all domains with finite volume.

Integration of this formula gives
\[ S_{\sigma,d}(\Omega, \Lambda) = (1 + o(1)) \sigma \int_0^\Lambda (\Lambda - \tau)^{\sigma - 1} \frac{\omega d}{(2\pi)^d} \text{vol}(\Omega) \tau^{d/2} d\tau \]

\[ = (1 + o(1)) S_{\sigma,d}^{\text{cl}}(\Omega, \Lambda) \quad \text{as} \quad \Lambda \to +\infty \]

with the corresponding classical phase space average

\[ S_{\sigma,d}^{\text{cl}}(\Omega, \Lambda) := \int_{x \in \Omega} \int_{\xi \in \mathbb{R}^d} (\Lambda - |\xi|^2)^\sigma \frac{dx \cdot d\xi}{(2\pi)^d} = L_{\sigma,d}^{\text{cl}} \text{vol}(\Omega) \Lambda^{\sigma+d/2}, \]

\[ L_{\sigma,d}^{\text{cl}} := \frac{\Gamma(\sigma + 1)}{2^d \pi^{d/2} \Gamma(1 + \sigma + d/2)} = \sigma B \left( \sigma, 1 + \frac{d}{2} \right) L_{0,d}^{\text{cl}}. \]
Analogously it holds

\[
\begin{align*}
  s_{\sigma,d}(\Omega, \Lambda) &= (1 + o(1)) \sigma \int_0^\infty \tau^{\sigma - 1} \left( N - L_{0,d}^{cl} \frac{\text{vol}(\Omega) \tau^{d/2}}{\eta(\Omega, \tau)} \right) d\tau \\
  &= (1 + o(1)) s_{\sigma,d}^{cl}(\Omega, N) \quad \text{as} \quad N \to +\infty, \\
  s_{\sigma,d}^{cl}(\Omega, N) &= c(\sigma, d) (\text{vol}(\Omega))^{-\frac{2\sigma}{d}} N^{1+\frac{2\sigma}{d}},
\end{align*}
\]

with the asymptotical constant

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

\[
\#\{\lambda_k < \Lambda\} = n(\Omega, \Lambda) \leq r(0, d)\eta(\Omega, \Lambda), \quad \Lambda > 0,
\]

\[
\sum_k (\Lambda - \lambda_k)_+^\sigma = S^\sigma_{\sigma,d}(\Omega, \Lambda) \leq r(\sigma, d)S^{cl}_{\sigma,d}(\Omega, \Lambda), \quad \Lambda > 0,
\]

\[
\sum_{k=1}^N \lambda_k^\sigma = s^\sigma_{\sigma,d}(\Omega, N) \geq \rho(\sigma, d)S^{cl}_{\sigma,d}(\Omega, N), \quad N \in \mathbb{N}.
\]

Let us point out the following known information on the constants \(r\) and \(\rho\):

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

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

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

\[
n(\Omega, \Lambda) = \underbrace{L_{0,d}^{cl} \text{vol}(\Omega) \Lambda^{d/2}}_{\eta(\Omega,\Lambda)} - \frac{1}{4} L_{0,d-1}^{cl} \partial \Omega \Lambda^{(d-1)/2} + o(\Lambda^{(d-1)/2})
\]

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 \( N \to +\infty \).
\[ S_{\sigma,d}(\Omega, \Lambda) = \frac{L_{\sigma,d}^{\text{cl}} \text{vol}(\Omega) \Lambda^{\sigma+d/2}}{S_{\sigma,d}^{\text{cl}}(\Omega, \Lambda)} - \frac{1}{4} L_{\sigma,d-1}^{\text{cl}} |\partial\Omega| \Lambda^{\sigma+(d-1)/2} + o(\Lambda^{\sigma+(d-1)/2}), \]

\[ s_{\sigma,d}(\Omega, N) = \frac{c(\sigma, d) (\text{vol}(\Omega))^{-\frac{2\sigma}{d}} N^{1+\frac{2\sigma}{d}}}{s_{\sigma,d}^{\text{cl}}(\Omega, N)} + \frac{L_{\sigma,d-1}^{\text{cl}} (L_{\sigma,d}^{\text{cl}})^{-1}}{4 \left( \frac{d-1}{2} + \sigma \right)} \cdot \frac{\sigma |\partial\Omega|}{(\text{vol}(\Omega))^{1+\frac{2\sigma-1}{d}}} N^{1+\frac{2\sigma-1}{d}} + o(N^{1+\frac{2\sigma-1}{d}}). \]

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

\[ S_{\sigma,d}(\Omega, \Lambda) \leq S_{\sigma,d}^{\text{cl}}(\Omega, \Lambda) - C \cdot |\partial\Omega| \Lambda^{\sigma+\frac{d-1}{2}} \text{ must fail!} \]
5. The Melas bound

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

$$\sum_{k=1}^{N} \lambda_k = s_{1,d}(\Omega, N) \geq c(1, d) \left( \operatorname{vol}(\Omega) \right)^{-\frac{2}{d}} N^{1+\frac{2}{d}} + M(d) \frac{\operatorname{vol}(\Omega)}{J(\Omega)} N$$

where

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

is the momentum of $\Omega$ 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 $\kappa(x', \Lambda)$. Put

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

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

That means $\Omega_\Lambda$ is the subset of $\Omega$, where the intervals of $\Omega$ in $x_d$-direction are longer than $l_\Lambda$. The set $\Omega_\Lambda$ is increasing in $\Lambda$.

The value $d_\Lambda(\Omega)$ is an effective measure of the projection of $\Omega_\Lambda$ on the $x'$-plane counting the number of sufficiently long intervals. It increases in $\Lambda$. 
For any open domain $\Omega \subset \mathbb{R}^d$, $\sigma \geq 3/2$ and any $\Lambda > 0$ it holds

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

**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 $\Omega_\Lambda$ and $d_\Lambda$: It counts the volume only where the domain is sufficiently wide for a bound state to settle.
- It works for $\Omega$ 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

\[ \nu \left( \sigma + \frac{d-2}{2}, 2 \right) \leq \nu(\sigma, d) \leq 2 \quad \text{and} \quad \nu(\sigma, 2) \geq 4\varepsilon(\sigma + 1/2) \]

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

\[ \sum_k (A^2 - k^2)^{\sigma + 1/2} \leq \frac{1}{2} B(\sigma + 3/2, 1/2)A^{2\sigma + 2} - \varepsilon(\sigma + 1/2)A^{2\sigma + 1}, \quad A \geq 1, \]

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

\[ 1.91 < \nu \left( \frac{3}{2}, 2 \right) \leq 2 \]
7. The key ingredient 1: Sharp Lieb-Thirring bounds for operator valued potentials

Let $G$ be an auxiliary Hilbert space. Consider a 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

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

Then it holds (Laptev, W.):

$$\text{tr}_{L^2(\mathbb{R}^m, G)} H^- \leq L^{cl}_{\sigma,m} \int \text{tr}_G W^{\sigma + \frac{m}{2}}_+(x) dx, \quad \sigma \geq 3/2.$$
8. The key ingredient 2: Induction in the dimension

We settle as an example the case of \(-\Delta^{\Omega}_{D}\) for \(d = 2\) and \(\sigma = 3/2\). A simple variational argument implies

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

where \(W(x) = \left( -\frac{d^2}{dy^2} \right)^{\Omega(x)}_{D} - \Lambda\) 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

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

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

We denote the set of such \( x \) by \( I_\Lambda \) and integration in the formula above takes place over the set \( I_\Lambda \) only.

Let us estimate the sum in the integrand for \( A > 1 \).
For $A > 1$ it holds

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

where $\delta$ 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 $\delta$ gives

$$\delta \approx 0.0210228223$$
This gives finally with \( l = l(x) \) and \( A = A(x) = l(x)l^{-1}_\Lambda = \pi^{-1}l(x)\Lambda^{1/2} \)

\[
S_{3/2,2}(\Omega, \Lambda) \leq \frac{3}{16} \int_{I_\Lambda} \frac{\pi^4}{l^4} \left( \frac{8}{15} \left( \frac{l\Lambda^{1/2}}{\pi} \right)^5 - \left( \frac{1}{2} - \delta \right) \left( \frac{l\Lambda^{1/2}}{\pi} \right)^4 \right) dx
\]

\[
= \frac{3}{16} \cdot \frac{8}{15} \cdot \frac{1}{\pi} \cdot \Lambda^{5/2} \int_{I_\Lambda} l(x) dx - \frac{3}{16} \left( \frac{1}{2} - \delta \right) \Lambda^2 \int_{I_\Lambda} dx
\]

\[
= L_{3/2,2}^{cl} \cdot \text{vol}(\Omega_\Lambda) \Lambda^{5/2} - (2 - 4\delta) \cdot \frac{1}{4} \cdot L_{3/2,1}^{cl} \cdot d_\Lambda \Lambda^2
\]

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

\[
L_{3/2,2}^{cl} = (10\pi)^{-1}, \quad L_{3/2,1}^{cl} = 3/16.
\]
10. Berezin-Li-Yau bounds for magnetic fields

Consider the magnetic Laplacian \((i\nabla + A(x))^2\) 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:

\[
S_{\sigma,d}(\Omega, \Lambda, A) \leq S_{\sigma,d}^{cl}(\Omega_\Lambda), \quad \sigma \geq 1, \quad \text{(Loss, Erdös, Wugalter)}
\]

if \(A\) 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?