Semiclassical bounds and beyond

- 1. The Setting of the Problem
- 2. Logarithmic Lieb-Thirring bounds
- 3. The Dirichlet Laplacian
- 4. Two-term spectral bounds
- 5. Some Application to the heat kernel

1. The setting of the Problem

Consider

$$H(V) = (-\Delta)^l - V(x) \quad \text{on} \quad L^2(\mathbb{R}^d), \quad l > 0.$$

If the potential $V(x)$ is sufficiently regular, the spectrum of H looks as follows

$$\sigma_{\text{ess}}(H) = [0, +\infty)$$

negative eigenvalues $\quad -\varkappa_j(V) < 0\,.$

We study counting functions and eigenvalue sums ($\sigma \geq 0$)

$$S_{\sigma,d,l}(V) = \sum_j (\varkappa_j(V))^\sigma = \mathrm{tr}(H(V))_-^\sigma$$

in comparison with the phase space average

$$S^{\mathrm{cl}}_{\sigma,d,l}(V) = \int\int (|\xi|^{2l} - V(x))_-^\sigma \frac{dx d\xi}{(2\pi)^d} = L^{\mathrm{cl}}_{\sigma,d,l} \int V_+^{\sigma+\frac{d}{2l}}(x) dx$$

1.1 Lieb-Thirring and Cwikel-Lieb-Rosenblum bounds - Estimates from above

Put $l > 0$. Then it holds

$$\mathrm{tr} H_-^\sigma = S_{\sigma,d,l}(V) \le R_{\sigma,d,l} S^{\mathsf{cl}}_{\sigma,d,l}(V) = L_{\sigma,d,l} \int V_+^{\sigma+\frac{d}{2l}}(x)\,dx$$

if and only if

$$\begin{array}{llllll} \sigma \ge \sigma_{\mathsf{crit}} & \text{if} & \sigma_{\mathsf{crit}} = 1 - \dfrac{d}{2l} > 0 & \text{that means} & d < 2l\,, \\ \sigma > 0 & \text{if} & \sigma_{\mathsf{crit}} = 1 - \dfrac{d}{2l} = 0 & \text{that means} & d = 2l\,, \\ \sigma \ge 0 & \text{if} & \sigma_{\mathsf{crit}} = 1 - \dfrac{d}{2l} < 0 & \text{that means} & d > 2l\,. \end{array}$$

1.2 Estimates from below

Assume that $V(x) \geq 0$, $l \in \mathbb{N}$ and $0 \leq \sigma \leq \sigma_{\text{crit}} = 1 - \frac{d}{2l}$. Then

$$\text{tr} H_-^\sigma = S_{\sigma,d,l}(V) \geq \tilde{R}_{\sigma,d,l} S^{\text{cl}}_{\sigma,d,l}(V) = \tilde{L}_{\sigma,d,l} \int V^{\sigma+\frac{d}{2l}}(x)dx.$$

Damanik-Remling $d = l = 1$; Grigoryan-Netrusov-Yau $d = 2l$; Geisinger $d < 2l$.

In particular, for $\sigma = \sigma_{\text{crit}} > 0$ a two-sided estimate holds true (Netrusov-W.)

$$\tilde{R}_{1-\frac{d}{2l},d,l} S^{\text{cl}}_{1-\frac{d}{2l},d,l}(V) \leq S_{1-\frac{d}{2l},d,l}(V) \leq R_{1-\frac{d}{2l},d,l} S^{\text{cl}}_{1-\frac{d}{2l},d,l}(V)$$

Open Problems

- The estimates from below in the critical and subcritical case are not settled for non-integer l.

- In particular, do Grigoryan-Netrusov-Yau bounds from below hold true for $l = d/2$, e.g. for $l = 1/2$ in the dimension $d = 1$?

1.3 Constants

For *all nice* potentials, and in the cases when the LTh holds true for *all* potentials with finite phase space average $S^{\mathrm{cl}}_{\sigma,d,l}(V)$, one has the Weyl asymptotic formula

$$S_{\sigma,d,l}(\alpha V) = (1 + o(1)) S^{\mathrm{cl}}_{\sigma,d,l}(\alpha V) \quad \text{as} \quad \alpha \to +\infty \,.$$

This implies the obvious estimate $R_{\sigma,d,l} \geq 1$. Moreover, the constants $R_{\sigma,d,l}$ are non-increasing in σ (Aizenman-Lieb).

There are various estimates from above on the values of $R_{\sigma,d,l}$ The sharp values for the constants $R_{\sigma,d,l} \geq 1$ are known in the cases

$$R_{\sigma,d,1} = 1 \quad \text{for all} \quad \sigma \geq \frac{3}{2} \quad \text{and} \quad d \in \mathbb{N} \, ; \qquad R_{\frac{1}{2},1,1} = 2 \,.$$

Open Problems

- Find the sharp values in any of the remaining cases, in particular for $d = 1$ and $\frac{1}{2} < \sigma < \frac{3}{2}$ and $\sigma = 1$ for arbitrary d.

- Find a direct approach to sharp constants in higher dimensions, that means without induction in the dimension! (Harrell-Stubbe)

- Find any sharp results in the higher order case! In the higher order case even the most natural conjectures seem to fail.

- Is the Lieb-Thirring hypothesis, namely that $R_{\sigma,d,l} = 1$ for all suitable large $\sigma \geq \sigma^*(d,l)$, somehow specifc for the case $l = 1$?

1.4 Some more on the critical case for higher orders

Put $d \geq 2l$ and $l \in \mathbb{N}$. Assume that $V(x) \geq 0$ is non-trivial and sufficiently nice. Then $(-\Delta)^l - \alpha V(x)$ has in the limit $\alpha \to 0+$ exactly

$$m(d,l) = \binom{l + \left[\frac{d}{2}\right]}{d} \quad \text{negative eigenvalues} \quad -\varkappa_1(\alpha V) \leq \ldots \leq -\varkappa_m(\alpha V) \,.$$

If $d > 2l$ they satisfy the weak coupling asymptotics

$$\begin{aligned}
\varkappa_1^{1-\frac{d}{2l}}(\alpha V) &= \alpha L^{(0)}_{d,l,1-\frac{d}{2l}} \int V(x)dx + o(\alpha) \quad \text{as} \quad \alpha \to 0+ \,, \\
\varkappa_j^{1-\frac{d}{2l}}(\alpha V) &= o(\alpha) \,, \quad j = 2, \ldots, m \quad \text{as} \quad \alpha \to 0+ \,.
\end{aligned}$$

1.5 Weak and Strong Coupling limits in the critical case

In the critical case $\sigma = \sigma_{\text{crit}} = 1 - \frac{d}{2l} > 0$ the order of weak and strong coupling asymptotics coincide

$$\begin{aligned} \operatorname{tr} H_-^{1-\frac{d}{2l}}(\alpha V) &= \alpha L^{(0)}_{d,l,1-\frac{d}{2l}} \int V(x)dx\,, \quad \alpha \to 0+\,, \\ \operatorname{tr} H_-^{1-\frac{d}{2l}}(\alpha V) &= \alpha L^{\text{cl}}_{d,l,1-\frac{d}{2l}} \int V(x)dx\,, \quad \alpha \to +\infty\,. \end{aligned}$$

The constant $L^{(0)}_{d,l,1-\frac{d}{2l}}$ corresponds to the Lieb-Thirring ratio for $V(x) = \delta(x)$. Moreover $L^{(0)}_{d,l,1-\frac{d}{2l}} > L^{\text{cl}}_{d,l,1-\frac{d}{2l}}$.

For $d = 1$, $l = 1$, $\sigma = \sigma_{\text{crit}} = 1/2$ we have in fact $L_{d,l,1-\frac{d}{2l}} = L^{(0)}_{d,l,1-\frac{d}{2l}}$. Here is $m(1,1) = 1$. The sharp Lieb-Thirring bound captures the weak coupling case!

Open Problem

This picture fails, generally speaking, in the higher order case!

Namely, for $d = 1$, $l = 2$, $\sigma = 3/4$ a subtle choice of a potential $V(x) = c_1\delta(x - x_1) + c_2\delta(x - x_2)$ shows that

$$L_{1,2,3/4} > L^{(0)}_{1,2,3/4}$$

by a tiny margin of (at least) 0.5% (Förster-Östensson). Here is $m(1,2) = 2$.

- Is for general $d < 2l$ the following true? Arazy-Zelenko?

$$\begin{aligned} L_{d,l,1-\frac{d}{2l}} &> L^{(0)}_{d,l,1-\frac{d}{2l}} \quad \text{iff} \quad m(d,l) \geq 2 \\ L_{d,l,1-\frac{d}{2l}} &= L^{(0)}_{d,l,1-\frac{d}{2l}} \quad \text{iff} \quad m(d,l) = 1 \end{aligned}$$

1.6 Important developments I will not talk about

- Better constants $L_{1,d,1}$ via mass transport (Eden-Foias, Dolbeault-Laptev-Loss)

$$R_{1,d,1} \leq 1.814$$

- Monotonicity in the coupling constant (Harrell-Stubbe)

$$S_{\sigma,d,1}(\alpha V)/S^{cl}_{\sigma,d,1}(\alpha V) \quad \text{is monotone increasing in} \quad \alpha \quad \text{for} \quad \sigma \geq 2$$

- Lieb-Thirring-Hardy bounds (Ekholm-Frank)

$$\operatorname{tr}\left(-\Delta - \frac{(d-2)^2}{4|x|^2} - V(x)\right)_-^\sigma \leq C(\sigma, d, \beta) \int V^{\sigma+\frac{d+\beta}{2}}(x)|x|^\beta dx$$

2. Logarithmic Bounds: The critical case for the counting function

Assume now $d = 2l$. Then $m(d, l) = 1$ and $\sigma_{\text{crit}} = 0$. According to Netrusov-Grigoryan-Yau we have the lower bound

$$\tilde{L}_{0,2l,l} \int V(x)dx \leq \text{card}\{-\varkappa_j < 0\} = S_{0,2l,l}(V)\,.$$

On the other hand, the corresponding upper bound

$$\text{card}\{-\varkappa_j < 0\} = S_{0,2l,l}(V) \leq L_{0,2l,l} \int V(x)dx\,.$$

must fail because of the weak coupling bound state:

For any non-trivial $V(x) \geq 0$ and any $\alpha > 0$ we have $1 \leq \text{card}\{-\varkappa_j < 0\}$ while $S^{\text{cl}}_{0,2l,l}(\alpha V) \to 0$ for $\alpha \to 0+$.

2.1 Non-Weyl strong coupling limits

There is a much deeper reason for the failure of the phase space bound, namely the non-Weyl strong coupling asymptotics:

Put $l = 1$ and $d = 2$. Then for $p > 1$ and $\alpha \to +\infty$ we know that with $r = |x|$

$$V_p^{(\infty)}(r) = \frac{\chi_{r>e^2}(r)}{r^2 |\ln r|^2 |\ln|\ln r||^{\frac{1}{p}}} \quad \text{implies} \quad \text{card}\{-\varkappa_j(\alpha V_p) < 0\} \asymp \alpha^p \,,$$

$$V_p^{(0)}(r) = \frac{\chi_{r<e^{-2}}(r)}{r^2 |\ln r|^2 |\ln|\ln r||^{\frac{1}{p}}} \quad \text{implies} \quad \text{card}\{-\varkappa_j(\alpha V_p) < -A < 0\} \asymp \alpha^p \,.$$

Note that $V_p^{(0)}, V_p^{(\infty)} \in L^1(\mathbb{R}^2)$. Since $S_{0,2,1}^{\text{cl}}(\alpha V) \sim \alpha$ even a bound

$$\text{card}\{-\varkappa_j < -A < 0\} \le B + C \int V(x)dx \quad \text{fails!}$$

2.2 Exponential weak coupling limits

We search for another critical bound following the motivation, that it should be determined by the weak coupling case:

For $d = 2$ and $l = 1$ one has

$$\ln \varkappa_1(\alpha V) \sim -\frac{4\pi}{\alpha \int V(x)dx} \quad \text{as} \quad \alpha \to 0+ \,.$$

Instead of looking in the power scale we search for the critical case of the upper bound in the logarithmic scale.

Therefore, we study eigenvalue sums $\sum_j F_s(\varkappa_j)$ with

$$F_s(t) = \frac{1}{|\ln ts^2|} \quad \text{as} \quad 0 < t \leq \frac{1}{es^2} \quad \text{and} \quad F_s(t) = 1 \quad \text{for} \quad 0 < \frac{1}{es^2} < t \,.$$

Note that $F_s(0+) = 0$.

2.3 Discussion of $\sum_j F_s(\varkappa_j)$

The weak coupling result reads now as follows

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

This supports the goal to estimate $\sum_j F_s(\varkappa_j)$ 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

$$\sum_j F_s(\varkappa_j(\alpha V_p^{(0)})) \sim \text{card}\left\{-\varkappa_j(\alpha V_p^{(0)}) < -\frac{1}{es^2}\right\} \asymp \alpha^p \quad \text{as} \quad \alpha \to 0\,.$$

Hence, a straightforward bound of $\sum_j F_s(\varkappa_j(\alpha V))$ by $\int V(x)dx$ is not possible.

2.4 The Main Result on Logarithmic LTh bounds

Put $d = 2$, $l = 1$ and $V \geq 0$. For $p > 1$ and $s > 0$ it holds

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

where the constants c_1 and c_p are independent of s and V.

If V is spherical symmetric, then exists a constant c_0, s.t.

$$\sum_j F_s(\varkappa_j) \leq c_1 \int_{|x|<s} V(x)|\ln|x|s^{-1}|dx + c_0 \|V\|_{L^1(\mathbb{R}^2)} .$$

Kowarik, Vugalter, W. in CMP 2007

2.5 Remarks on the logarithmic bounds

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

Remark 1. The r.h.s. is homogeneous of degree 1 in V. Hence, it reflects the correct order of the l.h.s. in the weak as well as in the strong coupling limit.

Remark 2. The finiteness of the r.h.s. excludes potentials $V = V_p^{(0)}$. This deals with the non-Weyl asymptotics of deep eigenvalues.

Remark 3. 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.

- Is there a similar bound for $\sqrt{-\frac{d^2}{dx^2}} - V(x)$ in the dimension $d = 1$?

3. The Dirichlet Laplacian

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

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.

3.1 Riesz means.

Along with the counting function we study the average spectral quantities

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

and

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

3.2 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

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

where

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

This formula holds for all domains with finite volume.

Integration of this formula gives

3.3 Weyl's law in the Berezin picture.

$$\begin{aligned} S_{\sigma,d}(\Omega,\Lambda) &= (1+o(1))\sigma \int_0^\Lambda (\Lambda-\tau)^{\sigma-1} \underbrace{\frac{\omega_d}{(2\pi)^d}\mathrm{vol}(\Omega)\tau^{d/2}}_{n^{cl}(\Omega,\tau)} d\tau \\ &= (1+o(1)) S^{cl}_{\sigma,d}(\Omega,\Lambda) \quad \text{as} \quad \Lambda \to +\infty \end{aligned}$$

with the corresponding classical phase space average

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

3.4 Weyl's law in the Li-Yau picture.

Analogously it holds

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

with the asymptotical constant

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

3.5 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:

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

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

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

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

3.6 Polya's conjecture

Polya conjectured that

$$r(0,d) = 1 \quad \text{for arbitrary domains, that means} \quad n(\Omega,\Lambda) \le n^{cl}(\Omega,\Lambda)$$

He proved it for tiling domains (from what follows $r(\sigma,d) = 1$ for any $\sigma > 0$ and tiling Ω's as well).

For general domains the problem remains too difficult so far, therefore lets change the setting and include a magnetic field: Consider the magnetic Laplacian

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

with Dirichlet boundary conditions on $\Omega \subset \mathbb{R}^d$. We shall simply put $\mathcal{A}$ in the notations introduced above.

Note that the magnetic field does not change the phase space volume.

3.7 Berezin-Li-Yau bounds for magnetic fields

So far there have been two result concerning sharp constants for magnetic fields:

(1) if $\mathcal{A}$ induces a *constant* magnetic field, then

$$S_{\sigma,d}(\Omega,\Lambda;\mathcal{A}) \le S^{cl}_{\sigma,d}(\Omega,\Lambda), \quad \sigma \ge 1,$$

(Erdös, Loss, Vougalter).

(2) if $\mathcal{A}$ induces an *arbitrary* magnetic field, then

$$S_{\sigma,d}(\Omega,\Lambda,\mathcal{A}) \le S^{cl}_{\sigma,d}(\Omega,\Lambda), \quad \sigma \ge \frac{3}{2},$$

since the classical constant holds true in Lieb-Thirring bounds with magnetic fields (Helffer, Laptev-W.)

3.8 Polya's conjecture fails for magnetic fields!

Let $\mathcal{A} = \frac{B}{2}(x_2, -x_1)$ induce a *constant* magnetic field. For $d = 2$ it holds (Frank-Loss-W. 08)

$$S_{\sigma,2}(\Omega, \Lambda, \mathcal{A}) \leq R_\sigma S^{cl}_{\sigma,2}(\Omega, \Lambda), \quad 0 \leq \sigma < 1,$$

where the constant

$$R_\sigma = 2\left(\frac{\sigma}{1+\sigma}\right)^\sigma > 1 \quad \text{for} \quad 0 \leq \sigma < 1$$

does not depend on B.

If one requires independence on B, this constant is optimal and cannot be improved for any given domain - not even for tiling domains! The example is provided on squares connecting the size of the square with the strength of the magnetic field properly.

3.9 Lessons to be learned

Lesson 1: You cannot prove Polya's original conjecture with methods that survive in the magnetic case.

Lesson 2: Polya's proof is not about phase space volume but about the density of states.

Indeed, for $0 \leq \sigma < 1$, $\mathcal{A} = \frac{B}{2}(x_2, -x_1)$ and tiling Ω it holds

$$\begin{aligned} S_{\sigma,2}(\Omega, \Lambda, \mathcal{A}) &\leq \mathfrak{B}_\sigma(B, \Lambda)\mathrm{vol}(\Omega)\,, \\ \mathfrak{B}_\sigma(B, \Lambda) &= \frac{B}{2\pi}\sum_{k\geq 0}(\Lambda - B(2k+1))_+^\sigma\,, \end{aligned}$$

and the constant $\mathfrak{B}_\sigma(B, \Lambda)$ is sharp.

Note that for $\sigma = 0$ the quantity $\mathfrak{B}_0(B, \Lambda)$ is just the density of states of the Landau Hamiltonian!

- Is this true for general domains?

4. Two-term Spectral Bounds

Weyl conjectured also a two-term asymptotical formula as $\Lambda \to +\infty$:

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

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

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

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

This formula holds for n under certain geometrical conditions on the domain (Ivrii); starting from $\sigma \geq 1$ these geometrical conditions can be dropped.

4.1 Statement of the Problem

Can on find universal bounds on the spectral quantities that

1. contain the sharp first Weyl term
2. *and* reflect the contribution of the second order term?

First note that any bound

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

must fail in general!

One must replace $|\partial\Omega|$ by some other geometric value.

4.2 The Melas bound

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

$$
\begin{aligned}
\sum_{k=1}^{N} \lambda_k &= s_{1,d}(\Omega, N) \geq \underbrace{c(1,d)\,(\mathrm{vol}(\Omega))^{-\frac{2}{d}}\, N^{1+\frac{2}{d}}}_{s^{cl}_{1,d}(\Omega,N)} + M(d)\frac{\mathrm{vol}(\Omega)}{J(\Omega)} N \\
\sum_{k} (\Lambda - \lambda_k)_+ &= S_{1,d}(\Omega, \Lambda) \leq S^{cl}_{1,d}\left(\Omega, \Lambda - M_d \frac{\mathrm{vol}(\Omega)}{J(\Omega)}\right) \\
J(\Omega) &= \min_{y \in \mathbb{R}^d} \int_{\Omega} |x - y|^2 dx
\end{aligned}
$$

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

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

4.3 Preparing the domain

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.

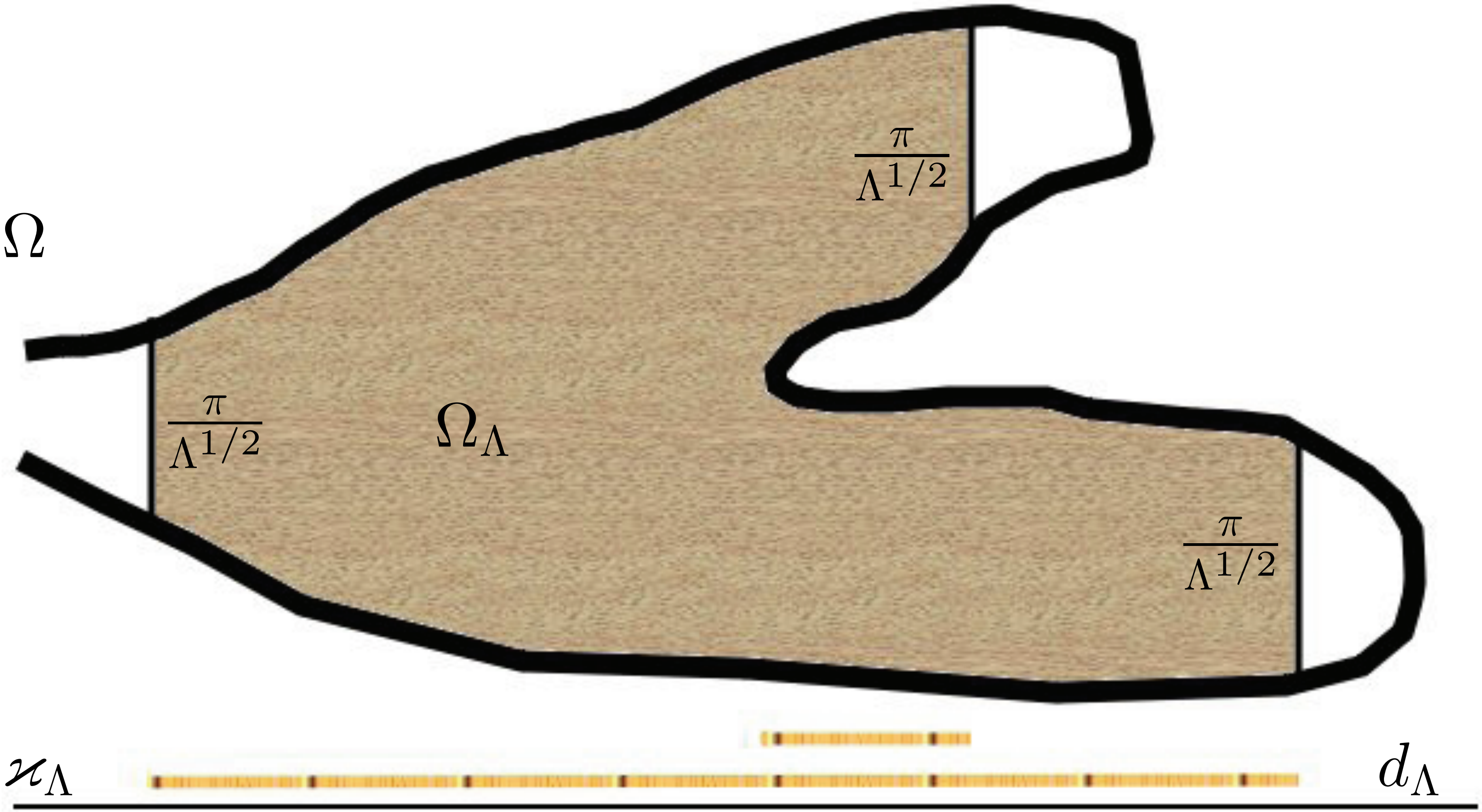
Let $\Omega_\Lambda(x')$ be the (finite) union of all such intervals, which are longer than $l_\Lambda := \pi \Lambda^{-1/2}$. The number of these intervals is denoted by $\varkappa(x', \Lambda)$. Put

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

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

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.


$\frac{\pi}{\Lambda^{1/2}}$
Ω
$\frac{\pi}{\Lambda^{1/2}}$
Ω_Λ
$\frac{\pi}{\Lambda^{1/2}}$
$\varkappa_\Lambda$
d_Λ

4.4 Statement of the Result

For any open domain $\Omega \subset \mathbb{R}^d$, $\sigma \geq 3/2$ and any $\Lambda > 0$ it holds (W. 2007)

$$S_{\sigma,d}(\Omega,\Lambda) \leq \underbrace{L^{cl}_{\sigma,d}\mathrm{vol}(\Omega_\Lambda)\Lambda^{\sigma+\frac{d}{2}}}_{S^{cl}_{\sigma,d}(\Omega_\Lambda;\Lambda)} - \nu(\sigma,d)4^{-1}L^{cl}_{\sigma,d-1}d_\Lambda(\Omega)\Lambda^{\sigma+\frac{d-1}{2}}$$

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.
- In particular, it works for Ω of infinite volume as long as $\mathrm{vol}(\Omega_\Lambda)$ is finite.
- The result remains true for the case of arbitrary magnetic fields.

Bad:

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

4.5 Constants

For the constant we have

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

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

In particular,

$$\varepsilon(\sigma) = \frac{1}{2}B\left(\sigma+1, \frac{1}{2}\right), \quad \sigma \geq 3,$$

and e.g. for $\sigma = \frac{3}{2}$, $d = 2$ numerics gives $1.91 < \nu\left(\frac{3}{2}, 2\right) \leq 2\,.$

4.6 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.):

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

4.7 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

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

4.8 Applying the Lieb-Thirring inequality for operator valued potentials

The Lieb-Thirring inequality for operator valued potentials implies now

$$
\begin{aligned}
S_{3/2,2}(\Omega,\Lambda) &\le \operatorname{tr}\left(-\frac{d^2}{dx^2}-W_-(x)\right)_-^{3/2} \\
&\le \frac{3}{16}\int_{\mathbb{R}} \operatorname{tr} W_-^2(x)dx \le \frac{3}{16}\int_{\mathbb{R}}\sum_k(\Lambda-\pi^2k^2l^{-2}(x))_+^2 dx \\
&\le \frac{3}{16}\int_{I_\Lambda}\frac{\pi^4}{l^4(x)}\sum_{k=1}^{[A(x)]}(A^2(x)-k^2)^2 dx \\
&\le \frac{3}{16}\int_{I_\Lambda}\frac{\pi^4}{l^4(x)}\left(\frac{8}{15}A^5(x)-\varepsilon(2)A^4(x)\right)dx
\end{aligned}
$$

where $A(x)=l(x)l_\Lambda^{-1}$. Note that integration takes only place on the set $I_\Lambda\subset\mathbb{R}$ where $A(x)>1$ or equivalently $l(x)>l_\Lambda$.

4.9 Closing the argument

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

We use that $A = A(x) = l(x)l_\Lambda^{-1} = l(x)\Lambda^{1/2}/\pi$ and

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

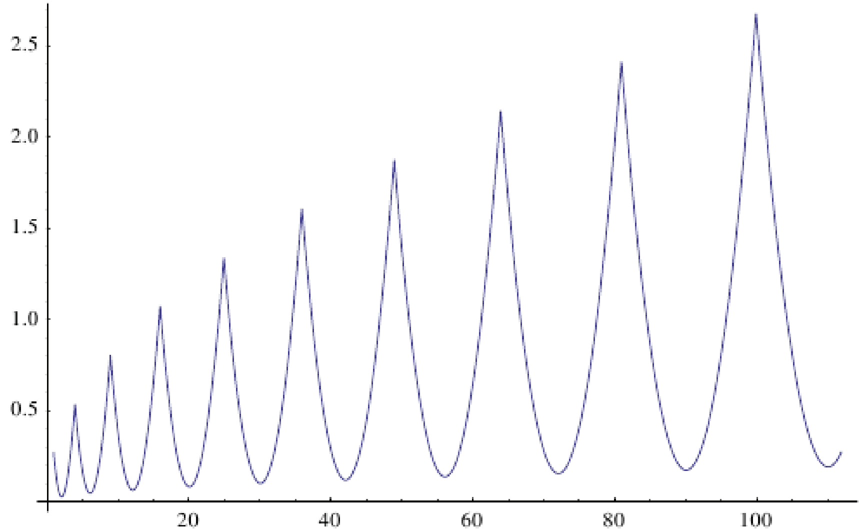
A modification with Hardy type terms

Let $I \subset \mathbb{R}$ be an open interval and $\sigma \geq 1$. Then for all $\Lambda > 0$

$$\text{Tr}\left(-\frac{d^2}{dt^2} - \Lambda\right)_-^{\sigma} \leq L^{cl}_{\sigma,1} \int_I \left(\Lambda - \frac{1}{4\delta(t)^2}\right)_+^{\sigma+1/2} dt \,,$$

$$f(\Lambda) = L^{cl}_{1,1} \int_0^{\pi} \left(\Lambda - \frac{1}{4\,\delta(t)^2}\right)_+^{3/2} dt - \sum_k (\Lambda - k^2)_+$$

is plotted for $1 < \Lambda < 112$, so that the first ten minima are shown.



For an arbitrary direction $u \in \mathbb{S}^{d-1}$ and $x \in \Omega$ set

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

Let $u \in \mathbb{S}^{d-1}$ and $\sigma \geq 3/2$. Then for all $\Lambda > 0$ we have

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

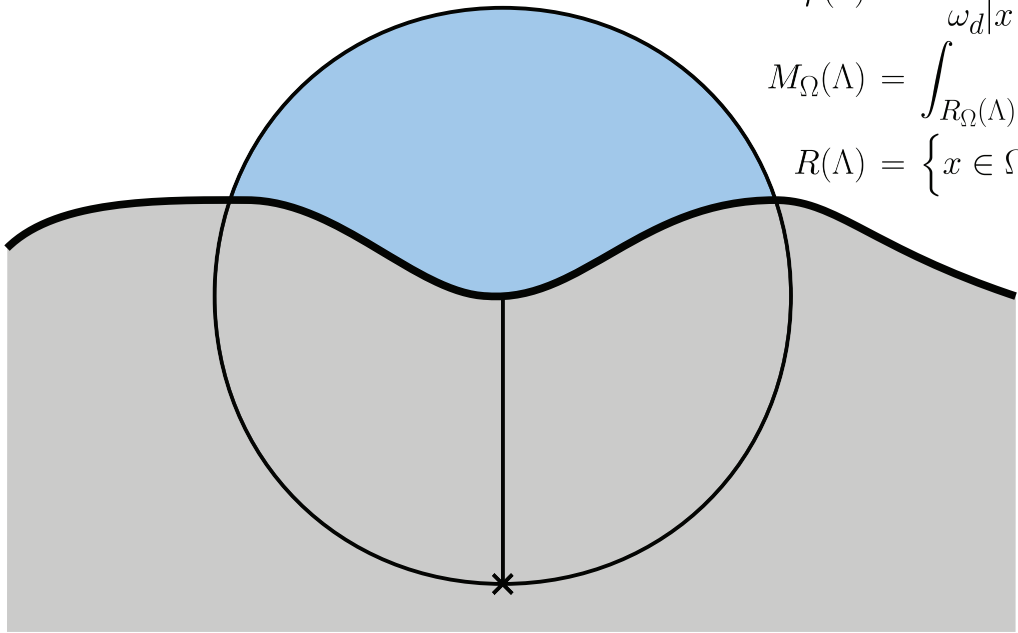
(Geisinger-Laptev-W. 2010)

4.10 A more geometric version

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

$$M_\Omega(\Lambda) = \int_{R_\Omega(\Lambda)} \rho(x)\, dx$$

$$R(\Lambda) = \left\{ x \in \Omega \,:\, \delta(x) < 1/(4\sqrt{\Lambda}) \right\}$$



Let $\Omega \subset \mathbb{R}^d$ be an open set with finite volume and $\sigma \geq 3/2$. Then for all $\Lambda > 0$ we have (Geisinger-Laptev-W. 2010)

$$S_{\sigma,d}(\Omega, \Lambda) \leq L^{cl}_{\sigma,d} |\Omega| \Lambda^{\sigma+d/2} - L^{cl}_{\sigma,d} 2^{-d+1} \Lambda^{\sigma+d/2} M_\Omega(\Lambda) .$$

4.11 What is the Melas bound about?

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 $F(\xi) = \sum_{j=1}^N |\hat{\psi}_j(\xi)|^2 \geq 0$. Then

$$\sum_{j=1}^N \lambda_j = \int_{\mathbb{R}^d} |\xi|^2 F(\xi) d\xi = I(F) \quad (1)$$

$$\int F(\xi) d\xi = N, \quad (2)$$

$$F(\xi) = \sum_{j=1}^N |\hat{\psi}_j(\xi)|^2 \leq (2\pi)^{-d} \|e^{i\xi x}\|^2_{L^2(\Omega)} = (2\pi)^{-d} \mathrm{vol}(\Omega)\,. \quad (3)$$

An estimate of $\sum_{j=1}^N \lambda_j$ from below can be obtained minimizing $I(F)$ for $F \geq 0$ satisfying (2) and (3).

4.12 Li-Yau, Melas and beyond.

A minimizer should be spherical symmetric and non-increasing in the radius. A straightforward bathtube principle gives the Li-Yau bound.

Melas puts forward the additional information $|\nabla F| \le 2(2\pi)^{-d}\sqrt{J(\Omega)\text{vol}(\Omega)}$. This gives an improvement of the bound.

But that is picking the wrong fight. The true remainder term is hidden in Bessel's inequality $F(\xi) = \sum_{j=1}^{N} |\hat{\psi}_j(\xi)|^2 \le (2\pi)^{-d}\text{vol}(\Omega)$.

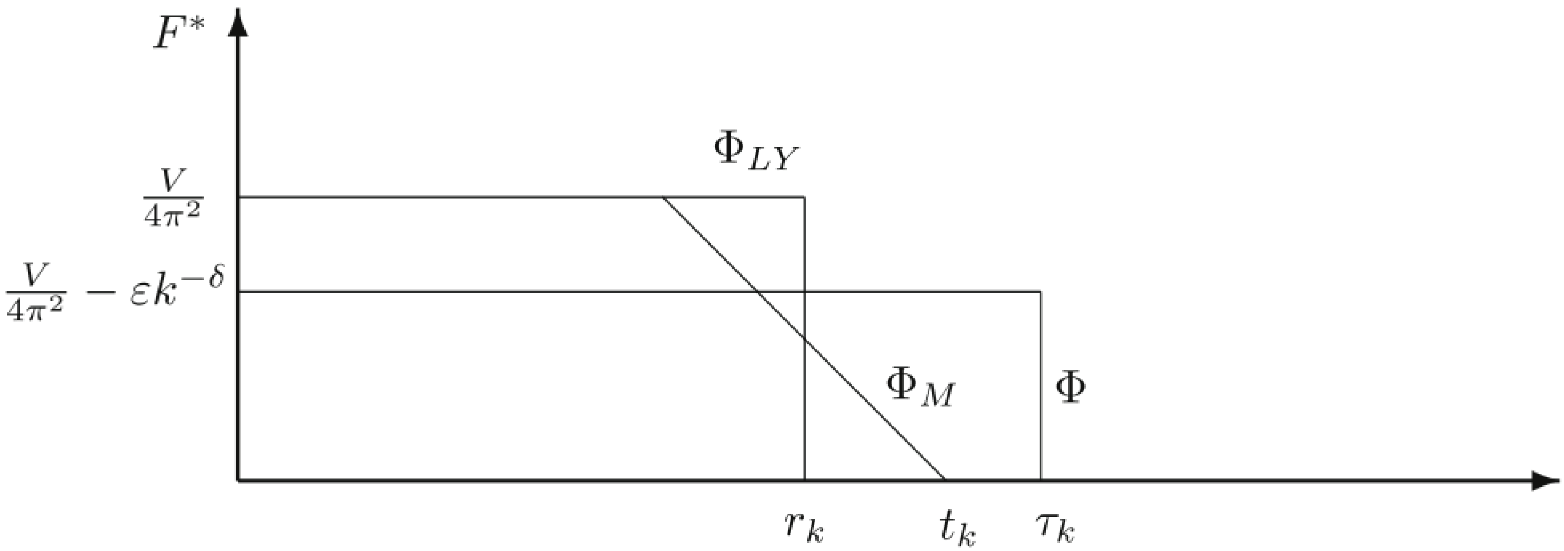


Fig. 1. Minimizers of the functional $\int_{\mathbb{R}^2} |\xi|^2 F^*(|\xi|)\, d\xi$

4.13 What about $\sigma = 1$?

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 $V = \mathrm{vol}(\Omega)$. Then for any $k \in \mathbb{N}$ and any $\alpha \in [0,1]$ we have (Kovarik-Vugalter-W.)

$$\sum_{j=1}^{k} \lambda_j \geq \frac{2\pi}{V} k^2 + \frac{4\alpha\, c_3}{V^{\frac{3}{2}}} k^{\frac{3}{2}-\epsilon(k)} \sum_{j=1}^{n} l_j \,\Theta\left(k - \frac{9V}{2\pi\, d_j^2}\right) + (1-\alpha)\frac{V}{32\, I} k,$$

where d_j is the distance of the middle third of p_j to $\partial\Omega \setminus p_j$

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

Open Problems

- Do the bounds

$$
\begin{aligned}
S_{1,d}(\Omega,\Lambda) &\leq S^{cl}_{1,d}(\Omega_\Lambda,\Lambda)\,,\\
S_{1,d}(\Omega,\Lambda) &\leq S^{cl}_{1,d}(\Omega,\Lambda) - \nu(1,d)L^{cl}_{1,d-1}d_\Lambda(\Omega)\Lambda^{1+\frac{d-1}{2}}\,,\\
S_{1,d}(\Omega,\Lambda) &\leq S^{cl}_{1,d}(\Omega_\Lambda,\Lambda) - \nu(1,d)L^{cl}_{1,d-1}d_\Lambda(\Omega)\Lambda^{1+\frac{d-1}{2}}
\end{aligned}
$$

hold true?

Note that $S_{\sigma,d}(\Omega,\Lambda) \leq R(\sigma,d)S^{cl}_{\sigma,d}(\Omega_\Lambda,\Lambda)$ is obvious for $\sigma \geq 1/2$.

- Is there a Melas type bound in the case of a (constant) magnetic field? (Our bounds extend to arbitrary magnetic fields for $\sigma \geq 3/2$.)

- What happens to the classical Berezin bound for $1 \leq \sigma < \frac{3}{2}$ in the case of arbitrary magnetic fields?

5 Some Applications to the Heat kernel

Using the monotonicity of the Laplace transformation

$$\begin{aligned}\mathcal{L}[f](t) &= \int_0^\Lambda f(\Lambda)e^{-t\Lambda}d\Lambda\,,\\ \mathcal{L}[(\Lambda-\lambda)_+^\sigma](t) &= e^{-t\lambda}t^{-\sigma-1}\Gamma(\sigma+1), \quad t>0\,,\end{aligned}$$

the Berezin bound (for any $\sigma \geq 1$) implies

$$\begin{aligned}Z(t) = \mathrm{tr}\; e^{\Delta t} &= \sum_k e^{-\lambda_k t} = \sum_k \frac{t^{\sigma+1}}{\Gamma(\sigma+1)}\mathcal{L}[(\Lambda-\lambda_k)_+^\sigma](t)\\ &= \frac{t^{\sigma+1}}{\Gamma(\sigma+1)}\mathcal{L}[S_{\sigma,d}(\Omega,\Lambda)](t) \leq \frac{t^{\sigma+1}}{\Gamma(\sigma+1)}\mathcal{L}[S_{\sigma,d}^{cl}(\Omega,\Lambda)](t)\end{aligned}$$

5.1 Kac' inequality

From this we get

$$Z(t) \leq \frac{t^{\sigma+1}}{\Gamma(\sigma+1)} L^{cl}_{\sigma,d} \mathrm{vol}(\Omega) \mathcal{L}[\Lambda^{\sigma+d/2}](t)$$

$$= \frac{t^{\sigma+1}}{\Gamma(\sigma+1)} \cdot \frac{\Gamma(\sigma+1)}{2^d \pi^{d/2} \Gamma(1+\sigma+d/2)} \cdot \mathrm{vol}(\Omega) \Gamma(1+\sigma+d/2) t^{-1-\sigma-d/2}$$

This implies Kac' inequality

$$Z(t) \leq \frac{\mathrm{vol}(\Omega)}{(4\pi t)^{d/2}} \quad \text{for any} \quad t > 0\,.$$

5.2 Improvements of Kac' bound (Harrell-Hermi)

$$S_{1,d}(\Omega,\Lambda) \le S^{\mathrm{cl}}_{1,d}\left(\Omega, \Lambda - M_d \frac{\mathrm{vol}(\Omega)}{J(\Omega)}\right)$$

implies that

$$Z(t) \le \frac{\mathrm{vol}(\Omega)}{(4\pi t)^{d/2}} e^{-M_d \frac{\mathrm{vol}(\Omega)}{J(\Omega)} t}$$

for any $t > 0$. Moreover, they conjectured that

$$Z(t) \le \frac{\mathrm{vol}(\Omega)}{(4\pi t)^{d/2}} e^{-M_d \frac{t}{(\mathrm{vol}(\Omega))^{2/d}}}, \quad t > 0\,.$$

5.3 Improvements of Kac' bound (Geisinger-W.)

Let $\lambda \in [\tilde{\lambda}, \lambda_1]$. For any $t > 0$ the bound

$$Z(t) \leq \frac{|\Omega|}{(4\pi t)^{\frac{d}{2}}} \hat{\Gamma}\left(\sigma_d + \frac{d}{2} + 1, \lambda t\right) - (R(t,\lambda))_+$$

holds true with a remainder term

$$R(t) = c_{1,d} \frac{|\Omega|^{\frac{d-1}{d}}}{(4\pi t)^{\frac{d-1}{2}}} \hat{\Gamma}\left(\sigma_d + \frac{d+1}{2}, \lambda t\right) - c_{2,d} \frac{|\Omega|^{\frac{d-3}{d}}}{(4\pi t)^{\frac{d-3}{2}}} \hat{\Gamma}\left(\sigma_d + \frac{d-1}{2}, \lambda t\right),$$

$$c_{1,d} = \frac{B\left(\frac{1}{2}, \sigma_d + \frac{d+1}{2}\right)}{2} \frac{\Gamma\left(\frac{d}{2}+1\right)^{\frac{d-1}{d}}}{\Gamma\left(\frac{d+1}{2}\right)}, \quad c_{2,d} = c_{1,d} \frac{2\pi^2 (d-1) \Gamma\left(\frac{d}{2}+1\right)^{-\frac{2}{d}}}{96(2\sigma_d + d - 1)}.$$

This beats the conjecture up to about $d = 633$.

5.4 Heat kernel asymptotics in unbounded domains

$$\Omega_f = \left\{(x,y) \in \mathbb{R}^2 : x \in \mathbb{R}\,,\ |y| < f(x)\right\} \quad \text{horn shaped}$$

Then for $t \to 0+$ one knowns that

$$\begin{aligned} Z(t;\Omega_{f_\mu}) &= \frac{\Gamma\left(1+\frac{\mu}{2}\right)\zeta(\mu)}{2\pi^{\mu+\frac{1}{2}}}\, t^{-\frac{\mu+1}{2}} + o\left(t^{-\frac{\mu+1}{2}}\right)\,, \\ f_\mu(s) &= s^{-\frac{1}{\mu}} \text{ with } \mu > 1\,, \end{aligned}$$

where $\zeta(\mu)$ is the Zeta function.

5.5 Heat kernel bounds in unbounded domains

Even just dropping the second order term from

$$\begin{aligned} Z(t) &= \frac{t^{\sigma+1}}{\Gamma(\sigma+1)}\mathcal{L}[S_{\sigma,d}(\Omega,\Lambda)] \\ &\leq \frac{t^{\sigma+1}}{\Gamma(\sigma+1)}\mathcal{L}[S^{cl}_{\sigma,d}(\Omega_\Lambda,\Lambda)]\,, \end{aligned}$$

one claims the result

$$Z(t;\Omega_{f_\mu}) \leq \frac{\Gamma\left(1+\frac{\mu}{2}\right)\zeta(\mu)}{2\pi^{\mu+\frac{1}{2}}}\,t^{-\frac{\mu+1}{2}} \quad \text{for all} \quad t>0 \quad \text{and} \quad \mu>1\,.$$