Spectral Theory and its Applications -
- Spectral and Functional Inequalities

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Lecture 4

• Schrödinger operators on $[0,\infty)$ with Robin boundary conditions.

Consider the equation with $V \geq 0$

$$-\psi'' - V\psi = -\lambda\,\psi, \qquad \psi'(0) = \mu\,\psi(0).$$

Theorem. (P.Exner, AL, M.Usman '14)

We obtain the inequality

$$\frac{3}{4}\,\mu\,\lambda_1 + \frac{1}{2}\,\lambda_1^{3/2} + \sum_{j=2}^{n} \lambda_j^{3/2} \leq \frac{3}{16}\int_0^\infty V^2\,dx + \frac{1}{4}\,\mu^3. \qquad (*)$$

Remark. Let $\mu = 0$ (Neumann problem). Then

$$\frac{1}{2}\,\lambda_1^{3/2} + \sum_{j=2}^{n} \lambda_j^{3/2} \le \frac{3}{16} \int_0^\infty V^2\,dx.$$

Remark. Let $V \equiv 0$ and $\mu < 0$. Then

$$-\psi'' = -\lambda\psi, \qquad \psi'(0) = \mu\psi(0).$$

The Robin boundary condition creates only one eigenfunction with negative eigenvalue

$$\psi(x) = e^{-\sqrt{\lambda}x}, \quad \text{where} \quad -\sqrt{\lambda} = \mu.$$

The inequality $(*)$ becomes equality

$$-\frac{3}{4}\,\lambda^{3/2} + \frac{1}{2}\,\lambda^{3/2} = -\frac{1}{4}\,\lambda^{3/2}.$$

Recently Lukas Schimmer has obtained a different inequality by using the so-called the double commutation method:

Theorem. For any $V \in L^2(\mathbb{R}_+)$, $V \geq 0$, the negative eigenvalues $-\lambda_j$ of $-d^2/dx^2 - V$ with Robin boundary condition $\varphi'(0) - \sigma_0\varphi(0) = 0$ satisfy

$$\sum_j \lambda_j^{3/2} \leq \frac{3}{16}\int_0^\infty V^2\, dx - \frac{3}{4}\sum_j \lambda_j(\sigma_{j-1} - \sigma_j) + \frac{1}{4}(\sigma_{j-1}^3 - \sigma_j^3),$$

where

$$\sigma_j = \sigma_{j-1} + \frac{|\varphi_j'(0)|^2}{\|\varphi_j\|^2}$$

with φ_j denoting the eigenfunction to λ_j.

Corollary.
For any $V \in L^2(\mathbb{R}_+)$, $V \geq 0$, the negative eigenvalues $-\lambda_j$ of $-d^2/dx^2 - V$ with Dirichlet boundary condition $\varphi(0) = 0$ satisfy

$$\sum_j \lambda_j^{3/2} \leq \frac{3}{16}\int_0^\infty V^2\, dx - \frac{3}{4}\sum_j \frac{|\varphi_j'(0)|^2}{\|\varphi_j\|^2}.$$

- The sum of the square roots.

Theorem. (D.Hundertmark, E.Lieb and L.Thomas)
Let $d = 1$ and $\gamma = 1/2$. Then the negative eigenvalues $\{-\lambda_k\}$ of the operator $\mathcal{H} = -\frac{d^2}{dx^2} - V$, satisfy

$$\sum_k \sqrt{\lambda_k} \leq \frac{1}{2} \int_{\mathbb{R}} V_+ \, dx.$$

In order to prove this statement we need to prove some auxiliary results.

- Properties of self-adjoint compact operators.

Denote by $\mu_n = \mu_n(A)$ eigenvalues of a compact, self-adjoint operator A.

Proposition. Let A be a compact, self-adjoint operator. Then for any $N \in \mathbb{N}$ the sum of its highest eigenvalues

$$|||A|||_N = \sum_{n=1}^{N} |\mu_n(A)|$$

is a norm. In particular, if A and B are compact, self-adjoint operators, then for any N we have

$$|||A + B|||_N \leq |||A|||_N + |||B|||_N.$$

- Birman–Schwinger principle.

Let $-\lambda$ be the eigenvalue of $-\Delta - V$, $V \geq 0$. Then there is ψ s.t.

$$-\Delta\psi - V\psi = -\lambda\psi \;\Rightarrow\; -\Delta\psi + \lambda\psi = V\psi \;\Rightarrow\; \psi = (-\Delta + \lambda)^{-1} V\psi.$$

- A modified Birman–Schwinger operator.

Let $0 \leq W \in L^2(\mathbb{R})$. For $\varepsilon > 0$ we consider the operator

$$\mathcal{L}_\varepsilon := 2\varepsilon\, W \left(-\frac{d^2}{dx^2} + \varepsilon^2\right)^{-1} W, \qquad \text{in} \quad L^2(\mathbb{R}).$$

Note that $\mathcal{L}_\varepsilon \geq 0$ and

$$2\varepsilon \left(-\frac{d^2}{dx^2} + \varepsilon^2\right)^{-1} = 2\pi\, \mathcal{F}^* g_\varepsilon \mathcal{F},$$

where $\mathcal{F}$ denote the Fourier transform and where

$$g_\varepsilon(\xi) = \frac{\varepsilon}{\pi(\xi^2 + \varepsilon^2)}.$$

The function g_ε is a probability density, that is,

$$\int_{\mathbb{R}} g_\varepsilon(\xi)\, d\xi = 1 \qquad \forall \varepsilon > 0.$$

The operator $\mathcal{L}_\varepsilon \geq 0$ and

Lemma. For any $\varepsilon > 0$

$$\operatorname{Tr} \mathcal{L}_\varepsilon = \int_{\mathbb{R}} W^2 \, dx.$$

Proof. Let Q is the integral operator in $L^2(\mathbb{R})$ with integral kernel

$$Q(x,y) = \sqrt{2\varepsilon} \int_{\mathbb{R}} \frac{e^{i\xi(x-y)}}{(\xi^2+\varepsilon^2)^{1/2}} \frac{d\xi}{2\pi} W(y).$$

Clearly

$$\mathcal{L}_\varepsilon = Q^* Q.$$

Therefore

$$\begin{aligned} \operatorname{Tr} Q^* Q = \iint_{\mathbb{R}\times\mathbb{R}} |Q(x,y)|^2 \, dxdy &= 2\varepsilon \iint_{\mathbb{R}\times\mathbb{R}} \left| \int_{\mathbb{R}} \frac{e^{i\xi(x-y)}}{(\xi^2+\varepsilon^2)^{1/2}} \frac{d\xi}{2\pi} \right|^2 W(y)^2 \, dxdy \\ &= 2\varepsilon \iint_{\mathbb{R}\times\mathbb{R}} \frac{1}{(\xi^2+\varepsilon^2)} W(y)^2 \frac{d\xi}{2\pi} \, dy = \int_{\mathbb{R}} g_\varepsilon(\xi) \, d\xi \int_{\mathbb{R}} W(y)^2 \, dy. \end{aligned}$$

- A property of the operator $\mathcal{L}_\varepsilon$.

Let us denote by $U(\xi)$ the unitary in $L^2(\mathbb{R})$ operator of multiplication by the function $e^{-i\xi x}$.

Proposition. Let $0 < \varepsilon' \leq \varepsilon$. Then

$$\mathcal{L}_\varepsilon = \int_{\mathbb{R}} U^*(\xi)\mathcal{L}_{\varepsilon'}\, U(\xi)\, g_{\varepsilon-\varepsilon'}(\xi)\, d\xi.$$

Proof. The operator $\mathcal{L}_\varepsilon = 2\pi W \mathcal{F}^* g_\varepsilon \mathcal{F} W$ is an integral operator with integral kernel

$$\mathcal{L}_\varepsilon(x,y) = \int_{\mathbb{R}} W(x) e^{i\xi(x-y)} W(y)\, g_\varepsilon(\xi)\, d\xi.$$

Note that

$$\widehat{g_\varepsilon} = (\mathcal{F} g_\varepsilon)(x) = e^{-\varepsilon|x|}.$$

Therefore for $0 < \varepsilon' < \varepsilon$ we have

$$g_\varepsilon(\xi) = \mathcal{F}^{-1}\widehat{g_\varepsilon}(\xi) = \mathcal{F}^{-1}\left(\widehat{g_{\varepsilon'}}\, \widehat{g_{\varepsilon-\varepsilon'}}\right)(\xi) = \int_{\mathbb{R}} g_{\varepsilon'}(\xi-\eta) g_{\varepsilon-\varepsilon'}(\eta)\, d\eta.$$

This implies that the kernel of $\mathcal{L}_\varepsilon$ can be written as

$$\begin{aligned}
\mathcal{L}_\varepsilon(x,y) &= \int_{\mathbb{R}} W(x) e^{i\xi(x-y)} W(y)\, g_\varepsilon(\xi)\, d\xi \\
&= \int_{\mathbb{R}}\int_{\mathbb{R}} e^{i\eta(x-y)}\, W(x)\, e^{i(\xi-\eta)(x-y)}\, W(y)\, g_{\varepsilon'}(\xi-\eta) g_{\varepsilon-\varepsilon'}(\eta)\, d\eta\, d\xi \\
&= \int_{\mathbb{R}}\int_{\mathbb{R}} e^{i\eta(x-y)}\, W(x)\, e^{i\rho(x-y)}\, W(y)\, g_{\varepsilon'}(\rho) g_{\varepsilon-\varepsilon'}(\eta)\, d\rho d\eta \\
&= \int_{\mathbb{R}} e^{i\eta(x-y)}\, \mathcal{L}_{\varepsilon'}(x,y)\, g_{\varepsilon-\varepsilon'}(\eta)\, d\eta.
\end{aligned}$$

• Monotonicity lemma.

Let $\mu_n = \mu_n(\mathcal{L}_\varepsilon)$ be eigenvalues of $\mathcal{L}_\varepsilon$ arranged in non-increasing order and repeated according to multiplicities.

Lemma. Let $0 < \varepsilon' \le \varepsilon$. Then for any $N \in \mathbb{N}$ we have

$$|||\mathcal{L}_\varepsilon|||_N \le |||\mathcal{L}_{\varepsilon'}|||_N,$$

that is

$$\sum_{n=1}^N \mu_n(\mathcal{L}_\varepsilon) \le \sum_{n=1}^N \mu_n(\mathcal{L}_{\varepsilon'}).$$

Proof. Using the fact that $|||\cdot|||$ is a norm we find

$$|||\mathcal{L}_\varepsilon|||_N = \left|\left|\left|\int_{\mathbb{R}} U^*(\xi)\mathcal{L}_{\varepsilon'}\, U(\xi)\, g_{\varepsilon-\varepsilon'}\, d\xi\right|\right|\right|_N$$
$$\le \int_{\mathbb{R}} |||U^*(\xi)\mathcal{L}_{\varepsilon'}\, U(\xi)|||_N\, g_{\varepsilon-\varepsilon'}(\xi)\, d\xi = |||\mathcal{L}_{\varepsilon'}|||_N.$$

- Proof of $\sum_n \sqrt{\lambda_n} \leq \frac{1}{2} \int_{\mathbb{R}} V_+ \, dx$.

By the variational principle it suffices to prove the theorem for $V \geq 0$. In that case, we set $W = \sqrt{V} \in L^2(\mathbb{R})$.

Consider the Birman–Schwinger operator

$$\frac{1}{2\varepsilon} \mathcal{L}_\varepsilon = W \left(-\frac{d^2}{dx^2} + \varepsilon^2 \right)^{-1} W, \quad \varepsilon > 0.$$

Let $\mu_n(\mathcal{L}_\varepsilon)$ be the n's eigenvalue of $\mathcal{L}_\varepsilon$ and let $-\lambda_n = -\lambda_n(\mathcal{H})$ be the n's negative eigenvalue of $\mathcal{H} = -d^2/dx^2 - V$.

According to the Birman–Schwinger principle

$$1 = \frac{1}{2\sqrt{\lambda_n}} \mu_n \left(\mathcal{L}_{\sqrt{\lambda_n}} \right), \quad \forall n. \qquad (*)$$

We now show that

$$2 \sum_{n=1}^{N} \sqrt{\lambda_n} \leq \sum_{n=1}^{N} \mu_n \left(\mathcal{L}_{\sqrt{\lambda_N}} \right), \quad \forall N.$$

If $N = 1$ this follows from $(*)$. Let $N = 2$, then again from $(*)$ and also by applying Corollary we have

$$2(\sqrt{\lambda_1} + \sqrt{\lambda_2}) \le \mu_1\left(\mathcal{L}_{\sqrt{\lambda_1}}\right) + \mu_2\left(\mathcal{L}_{\sqrt{\lambda_2}}\right) \le \mu_1\left(\mathcal{L}_{\sqrt{\lambda_2}}\right) + \mu_2\left(\mathcal{L}_{\sqrt{\lambda_2}}\right).$$

Let $N = 3$. Then

$$\begin{aligned} 2(\sqrt{\lambda_1} + \sqrt{\lambda_2} + \sqrt{\lambda_3}) &\le \mu_1\left(\mathcal{L}_{\sqrt{\lambda_1}}\right) + \mu_2\left(\mathcal{L}_{\sqrt{\lambda_2}}\right) + \mu_3\left(\mathcal{L}_{\sqrt{\lambda_3}}\right) \\ &\le \mu_1\left(\mathcal{L}_{\sqrt{\lambda_2}}\right) + \mu_2\left(\mathcal{L}_{\sqrt{\lambda_2}}\right) + \mu_3\left(\mathcal{L}_{\sqrt{\lambda_3}}\right) \\ &\qquad \le \mu_1\left(\mathcal{L}_{\sqrt{\lambda_3}}\right) + \mu_2\left(\mathcal{L}_{\sqrt{\lambda_3}}\right) + \mu_3\left(\mathcal{L}_{\sqrt{\lambda_3}}\right). \end{aligned}$$

Repeating this N-times we obtain the claimed inequality

$$2\sum_{n=1}^{N} \sqrt{\lambda_n} \le \sum_{n=1}^{N} \mu_n\left(\mathcal{L}_{\sqrt{\lambda_N}}\right), \quad \forall N.$$

We conclude the proof of the theorem by computing the trace of $\mathcal{L}_{\sqrt{\lambda_N}}$

$$\begin{aligned} 2\sum_{n=1}^{N} \sqrt{\lambda_k} &\le \operatorname{Tr} \mathcal{L}_{\sqrt{\lambda_N}} = \int \mathcal{L}_{\sqrt{\lambda_N}}(x, y)\Big|_{x=y} dx \\ &= \int_{\mathbb{R}} \int_{\mathbb{R}} W(x) e^{i\xi(x-y)} W(y)\, g_\varepsilon(\xi)\, d\xi\Big|_{x=y} dx = \int_{\mathbb{R}} W(x)^2 dx = \int_{\mathbb{R}} V(x) dx. \end{aligned}$$

The proof is complete.

- L-Th inequality for $\gamma = 1$.

Let $\{\psi_j\}_{j=1}^n$ be in orthonormal system of function in $L^2(\mathbb{R})$ and let

$$\rho(x) = \sum_{j=1}^{n} \psi_j^2(x).$$

Theorem. (Eden and Foias inequality)

$$\int_{\mathbb{R}} \rho^3(x)\,dx = \int \Big(\sum_{j=1}^{n} |\psi_j(x)|^2\Big)^3 dx \le \sum_{j=1}^{n} \int_{\mathbb{R}} |\psi'_j(x)|^2\,dx.$$

Proof. We first derive a so-called Agmon inequality

$$\|\psi\|_{L^\infty} \le \|\psi\|_{L^2}^{1/2}\|\psi'\|_{L^2}^{1/2}.$$

Indeed

$$|\psi(x)|^2 = \frac{1}{2}\Big|\int_{-\infty}^{x} |\psi^2|'\,dt - \int_{x}^{\infty} |\psi^2|'\,dt\Big| \le \int |\psi||\psi'|\,dt \le \|\psi\|_{L^2}\|\psi'\|_{L^2}.$$

Let now $\xi = (\xi_1, \xi_2, \ldots, \xi_n) \in \mathbb{R}^n$. Then by Agmon-Kolmogorov inequality

$$\Big|\sum_{j=1}^{n} \xi_j\psi_j(x)\Big| \le \Big(\sum_{j,k=1}^{n} \xi_j\bar{\xi}_k(\psi_j,\psi_k)\Big)^{1/4}\Big(\sum_{j,k=1}^{n} \xi_j\bar{\xi}_k(\psi'_j,\psi'_k)\Big)^{1/4}$$

$$\le \Big(\sum_{j=1}^{n} \xi_j^2\Big)^{1/4}\Big(\sum_{j,k=1}^{n} \xi_j\bar{\xi}_k(\psi'_j,\psi'_k)\Big)^{1/4}.$$

So we have proved

$$\Big|\sum_{j=1}^{n}\xi_j\psi_j(x)\Big| \le \Big(\sum_{j=1}^{n}\xi_j^2\Big)^{1/4}\Big(\sum_{j,k=1}^{n}\xi_j\bar{\xi}_k(\psi_j',\psi_k')\Big)^{1/4}.$$

If we set $\xi_j = \psi_j(x)$ then the latter inequality becomes

$$\rho(x) = \sum_{j=1}^{n}|\psi_j(x)|^2 \le \rho^{1/4}(x)\Big(\sum_{j,k=1}^{n}\psi_j(x)\overline{\psi_k(x)}(\psi_j',\psi_k')\Big)^{1/4}.$$

Thus

$$\rho^3(x) \le \sum_{j,k=1}^{n}\psi_j(x)\overline{\psi_k(x)}(\psi_j',\psi_k').$$

Integrating both sides we arrive at

$$\int\Big(\sum_{j=1}^{n}|\psi_j(x)|^2\Big)^3\,dx \le \sum_{j=1}^{n}\int|\psi_j'|^2\,dx$$

and obtain the proof.

- Spectrum of Schrödinger operators.

Let $\{\psi_j\}_{j=1}^{\infty}$ be the orthonormal system of eigenfunctions corresponding to the negative eigenvalues of the Schrödinger operator

$$-\frac{d^2}{dx^2}\psi_j - V\,\psi_j = -\lambda_j\psi_j,$$

where we assume that $V \geq 0$. Then by using the latter result and Hölder's inequality we obtain

$$\int \Big(\sum_{j=1}^{n} |\psi_j(x)|^2\Big)^3 dx - \Big(\int V^{3/2}\,dx\Big)^{2/3} \int \Big(\sum_{j=1}^{n} |\psi_j(x)|^2\Big)^3 dx\Big)^{1/3}$$

$$\leq \sum_j \int \Big(|\psi_j'|^2 - V\,|\psi_j|^2\Big)\,dx = -\sum_j \lambda_j.$$

Denote

$$X = \Big(\int \Big(\sum_{j=1}^{n} |\psi_j(x)|^2\Big)^3 dx\Big)^{1/3}.$$

Then the latter inequality can be written as

$$X^3 - \left(\int V^{3/2}\,dx\right)^{2/3} X \le -\sum_j \lambda_j.$$

Maximizing the left hand side we find $X = \frac{1}{\sqrt{3}}\left(\int V^{3/2}\,dx\right)^{1/3}$. This implies

$$\frac{1}{3\sqrt{3}}\int V^{3/2}\,dx - \frac{1}{\sqrt{3}}\int V^{3/2}\,dx = -\frac{2}{3\sqrt{3}}\int V^{3/2}\,dx \le -\sum_j \lambda_j$$

and we finally obtain $\sum_j \lambda_j \le \frac{2}{3\sqrt{3}}\int V^{3/2}\,dx$.

Until recently it was the best known constant in Lieb-Thirring's inequality for $\gamma = 1$. It was improved by R.L. Frank, D. Hundertmark, M. Jex, P.T. Nam in any dimension.

Thank you