Spectral properties (e.g., selfadjointness, semiboundedness from below, discreteness property, discreteness and finiteness of negative spectrum, spectral types, etc.) of 1D-Schrodinger operators with point interactions.

Mark Malamud

Institute of Appl. Math. and Mech.

δ-interactions

Consider the Sturm–Liouville differential expression

$$\ell_V := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x), \quad x \in \mathcal{I} = (a,b) \subseteq \mathbb{R}. \tag{1}$$

Classical requirement: $V \in L^1_{\mathrm{loc}}(\mathcal{I})$.
The Kronig-Penney model [1931]: $V(x) = \sum_{n\in\mathbb{N}} \alpha\delta(x-n)$.
Rigorous treatment of δ-interactions:

$$\mathrm{H}_\alpha = -\frac{d^2}{dx^2} + \alpha\delta(x)$$

is defined in $L^2(\mathbb{R})$ as follows $\mathrm{H}_\alpha f = -f''$ on the domain

$$\mathrm{dom}\,(\mathrm{H}_\alpha) = \left\{ f \in W^{2,2}(\mathbb{R}\setminus\{0\}) : \begin{array}{l} f(+0) = f(-0) =: f(0), \\ f'(+0) - f'(-0) = \alpha f(0) \end{array} \right\}.$$

The operator H_α acts as $\mathrm{H}_\alpha = -f'' + \alpha\ f(0)\delta(x)$, where f'' is understood in the sense of distributions.

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Let $X = \{x_n\}_0^\infty \subset \mathbb{R}_+$ be a decreasing sequence of points, $x_0 = 0$, and $\{\alpha_n\}_1^\infty \subset \mathbb{R}$. Define the operator $\mathrm{H}^0_{X,\alpha}$ as

$$\tau := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} \tag{2}$$

on the domain

$$\operatorname{dom}(\mathrm{H}^0_{X,\alpha}) = \Big\{ f \in W^{2,2}_{comp}(\mathcal{I} \setminus X) : f'(0) = 0, \\ \begin{array}{c} f(x_n+) = f(x_n-) \\ f'(x_n+) - f'(x_n-) = \alpha_n f(x_n) \end{array}, \ n \in \mathbb{N} \Big\}. \tag{3}$$

Clearly, $\mathrm{H}^0_{X,\alpha}$ is symmetric. Denote by $\mathrm{H}_{X,\alpha} := \overline{\mathrm{H}^0_{X,\alpha}}$ its closure. The operator $\mathrm{H}_{X,\alpha}$ is called an operator with point δ-interactions at points x_n with intensities $\{\alpha_n\}_1^\infty$.

Boundary triplets for the operator $\mathrm{H}^*_{\min}$.

Set $d_k := x_k - x_{k-1}$. We will treat the operator $\mathrm{H}_{X,\alpha}$ as an extension of the following symmetric operator in $L^2(\mathbb{R}_+)$

$$\mathrm{H}_{\min} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \qquad \mathrm{dom}\,(\mathrm{H}_{\min}) = W^{2,2}_0(\mathbb{R}_+ \setminus X). \tag{4}$$

Clearly, $\mathrm{H}_{\min}$ is closed and

$$\mathrm{H}_{\min} = \oplus_{n=1}^{\infty} \mathrm{H}_n, \quad \text{where} \quad \mathrm{H}_n = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \quad \mathrm{dom}\,(\mathrm{H}_n) = W^{2,2}_0[x_{n-1}, x_n]. \tag{5}$$

A triplet $\widetilde{\Pi}_n = \{\mathbb{C}^2, \widetilde{\Gamma}^{(n)}_0, \widetilde{\Gamma}^{(n)}_1\}$ given by

$$\widetilde{\Gamma}^{(n)}_0 f := \begin{pmatrix} f(x_{n-1}+) \\ -f(x_n-) \end{pmatrix}, \quad \widetilde{\Gamma}^{(n)}_1 f := \begin{pmatrix} f'(x_{n-1}+) \\ f'(x_n-) \end{pmatrix}, \quad f \in W^2_2[x_{n-1}, x_n], \tag{6}$$

forms a boundary triplet for H^*_n satisfying $\ker(\widetilde{\Gamma}^{(n)}_0) = \mathrm{dom}\,(H^F_n)$, where $\mathrm{H}^{\mathrm{F}}_n$ is the Friedrichs' extension of H_n.

Theorem 3

Assume $d^* = \sup_{n\in\mathbb{N}} d_n < +\infty$, and define the mappings $\Gamma_j^{(n)} : W_2^2[x_{n-1}, x_n] \to \mathbb{C}^2$, $n \in \mathbb{N}$, $j \in \{0,1\}$, by setting

$$\Gamma_0^{(n)} f := \begin{pmatrix} d_n^{1/2} f(x_{n-1}+) \\ -d_n^{1/2} f(x_n-) \end{pmatrix}, \quad \Gamma_1^{(n)} f := \begin{pmatrix} \frac{d_n f'(x_{n-1}+) + (f(x_{n-1}+) - f(x_n-))}{d_n^{3/2}} \\ \frac{d_n f'(x_n-) + (f(x_{n-1}+) - f(x_n-))}{d_n^{3/2}} \end{pmatrix}. \tag{7}$$

Then:

(i) For any $n \in \mathbb{N}$ the triplet $\Pi_n = \{\mathbb{C}^2, \Gamma_0^{(n)}, \Gamma_1^{(n)}\}$ is a boundary triplet for H_n^*.

(ii) The direct sum $\Pi = \oplus_{n=1}^{\infty} \Pi_n$ is a boundary triplet for the operator $\mathrm{H}_{\min}^*$.

Connection with Jacobi matrices

Consider the semi-infinite Jacobi matrix

$$B_{X,\alpha} = \begin{pmatrix} r_1^{-2}\left(\alpha_1 + \frac{1}{d_1} + \frac{1}{d_2}\right) & -(r_1 r_2 d_2)^{-1} & 0 & \dots \\ -(r_1 r_2 d_2)^{-1} & r_2^{-2}\left(\alpha_2 + \frac{1}{d_2} + \frac{1}{d_3}\right) & -(r_2 r_3 d_3)^{-1} & \dots \\ 0 & -(r_2 r_3 d_3)^{-1} & r_3^{-2}\left(\alpha_3 + \frac{1}{d_3} + \frac{1}{d_4}\right) & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \tag{8}$$

where $r_n := \sqrt{d_n + d_{n+1}}, \ n \in \mathbb{N}$.

Basic Lemma

The (minimal) Jacobi operator $B_{X,\alpha}$ is the boundary operator for $\mathrm{H}_{X,\alpha}$ in the triplet $\Pi = \oplus_{n=1}^{\infty} \Pi_n$, i.e.

$$\mathrm{H}_{X,\alpha} = \mathrm{H}_{B_{X,\alpha}} = \mathrm{H}^*_{\min} \lceil \mathrm{dom}\,(\mathrm{H}_{B_{X,\alpha}}),$$

$$\mathrm{dom}\,(\mathrm{H}_{B_{X,\alpha}}) = \{f \in \mathrm{dom}\,(H^*_{\min}) : \Gamma_1 f = B_{X,\alpha}\Gamma_0 f\}.$$

Theorem 4

Assume $H_{X,\alpha}$ is the minimal symmetric operator associated with (1). Let also $B_{X,\alpha}$ be the minimal operator associated with the Jacobi matrix (8). Then:

(i) The deficiency indices of $H_{X,\alpha}$ and $B_{X,\alpha}$ are equal and

$$\mathrm{n}_{\pm}(H_{X,\alpha}) = \mathrm{n}_{\pm}(B_{X,\alpha}) \leq 1.$$

In particular, $H_{X,\alpha,q}$ is self-adjoint if and only if $B_{X,\alpha}$ is.

(ii) The operator $H_{X,\alpha}$ is lower semibounded if and only if so is the Jacobi operator $B_{X,\alpha}$.

In addition, assume that $H_{X,\alpha}$ (and hence $B_{X,\alpha}$) is self-adjoint. Then:

(iii) The operator $H_{X,\alpha}$ is nonnegative if and only if so is $B_{X,\alpha}$.

(iv) The total multiplicities of the negative spectra of $H_{X,\alpha}$ and $B_{X,\alpha}$ coincide:

$$\kappa_{-}(H_{X,\alpha}) = \kappa_{-}(B_{X,\alpha}). \tag{9}$$

Theorem 4

(v) For any $p \in (0, \infty]$, the following equivalence holds:

$$E_{H_{X,\alpha}}(\mathbb{R}_-)H_{X,\alpha} \in \mathfrak{S}_p \iff E_{B_{X,\alpha}}(\mathbb{R}_-)B_{X,\alpha} \in \mathfrak{S}_p.$$

In particular, the negative part of the spectrum $H_{X,\alpha}$ is discrete if and only if the same holds for the negative spectrum of $B_{X,\alpha}$.

(vi) $\sigma_c(H_{X,\alpha}) \subseteq [0, \infty)$ if and only if $\sigma_c\left(B_{X,\alpha}\right) \subseteq [0, \infty)$.

(vii) $\sigma_c(H_{X,\alpha}) \subset (0, \infty)$ if and only if $\sigma_c\left(B_{X,\alpha}\right) \subset (0, \infty)$.

($viii$) The operator $H_{X,\alpha}$ has purely discrete spectrum if and only if $\lim_{n\to\infty} d_n = 0$ and $B_{X,\alpha}$ has purely discrete spectrum.

(ix) Let $\widetilde{\alpha} = \{\widetilde{\alpha}_k\}_{k=1}^{\infty} \subset \mathbb{R}$, and let $B_{X,\widetilde{\alpha}}$ be the minimal operator associated with the matrix (8) and constructed by the sequence $\widetilde{\alpha}$ instead of α. If $H_{X,\widetilde{\alpha}} = H^*_{X,\widetilde{\alpha}}$ then $B_{X,\widetilde{\alpha}} = B^*_{X,\widetilde{\alpha}}$, and for any $p \in (0, +\infty]$ the following equivalence holds:

$$(H_{X,\alpha} - i)^{-1} - (H_{X,\widetilde{\alpha}} - i)^{-1} \in \mathfrak{S}_p \iff (B_{X,\alpha} - i)^{-1} - (B_{X,\widetilde{\alpha}} - i)^{-1} \in \mathfrak{S}_p.$$

Self-adjointness

Applying Carleman test to the Jacobi operator $B_{X,\alpha}$ and applying Theorem 4(i) we obtain the following result.

Proposition 5

$\mathrm{H}_{X,\alpha}$ is self-adj. for any $\alpha = \{\alpha_n\}_{n=1}^{\infty} \subset \mathbb{R}$ whenever

$$\sum_{n=1}^{\infty} d_n^2 = \infty. \tag{10}$$

Proposition 6

Let $\{d_n\}_{n=1}^{\infty} \in l_2$, $d_n \geq 0$, and $d_{n-1}d_{n+1} \geq d_n^2, \quad n \in \mathbb{N}$. If

$$\sum_{n=1}^{\infty} d_{n+1} \left| \alpha_n + \frac{1}{d_n} + \frac{1}{d_{n+1}} \right| < \infty, \tag{11}$$

then the operator $\mathrm{H}_{X,\alpha}$ is symmetric with $n_{\pm}(\mathrm{H}_{X,\alpha}) = 1$.

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Example 7

Let $\mathcal{I} = \mathbb{R}_+$, $x_0 = 0$, $x_n - x_{n-1} = d_n := 1/n$, $n \in \mathbb{N}$. (Clearly, $\{d_n\}_{n=1}^{\infty} \in l_2$.) Then:

(i) $n_{\pm}(\mathrm{H}_{X,\alpha}) = 0$ if $\sum_{n=1}^{\infty} \frac{|\alpha_n|}{n^3} = \infty$;

(ii) $n_{\pm}(\mathrm{H}_{X,\alpha}) = 0$ if $\alpha_n \le -4\big(n + \frac{1}{2}\big) + O(n^{-1})$;

(iii) $n_{\pm}(\mathrm{H}_{X,\alpha}) = 0$ if $\alpha_n \ge -\frac{C}{n}$, $n \in \mathbb{N}$, $C \equiv const > 0$;

(iv) $n_{\pm}(\mathrm{H}_{X,\alpha}) = 1$ if $\alpha_n = -2n - 1 + O(n^{-\varepsilon})$ with some $\varepsilon > 0$.

Proposition 8 (Lower semiboundedness)

The operator $\mathrm{H}_{X,\alpha}$ is lower semibounded if

$$\inf_{n \to \infty} \frac{\alpha_n}{d_{n-1} + d_n} > -\infty, \tag{12}$$

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Discreteness of spectrum

Applying Chihara's condition for the discreteness of spectra of Jacobi matrices, we obtain

Proposition 9

Let $X = \{x_n\}_{n=0}^{\infty} \subset \mathcal{I}$ and $\alpha = \{\alpha_n\}_{n\in\mathbb{N}} \subset \mathbb{R}$ be such that $\mathrm{H}_{X,\alpha} = \mathrm{H}_{X,\alpha}^*$, $\lim_{n\to\infty} d_n = 0$. If

$$\lim_{n\to\infty} \frac{|\alpha_n|}{d_{n+1}} = \infty, \qquad \lim_{n\to\infty} \frac{1}{d_n \alpha_{n-1}} > -\frac{1}{4} \quad \text{and} \quad \lim_{n\to\infty} \frac{1}{d_n \alpha_n} > -\frac{1}{4}, \tag{13}$$

then the operator $\mathrm{H}_{X,\alpha}$ has discrete spectrum.

Absolutely continuous of spectrum

Consider $\tau_q := -\frac{d^2}{dx^2} + q(x)$. Let $H_{X,\alpha,q}$ be the realization τ_q on (3). Applying Kato-Rozenblum theorem we obtain

Proposition 10

Assume that

$$\sum_{n=1}^{\infty} \frac{|\alpha_n|}{d_{n+1}} < \infty. \tag{14}$$

Then absolutely continuous part $H^{\mathrm{ac}}_{X,\alpha,q}$ of the Hamiltonian $H_{X,\alpha,q}$ is unitarily equivalent to the operator $H_q^N := H_{X,0,q}$ that is the Neumann realization of (2) in $L^2(\mathbb{R}_+)$. In particular,

$$\sigma_{ac}(H_{X,\alpha,q}) = \sigma_{ac}(H_q^N), \tag{15}$$

where $\mathrm{dom}\,(H_q^N) = \mathrm{dom}\,(H_{X,0,q}) \subset \{W^{2,2}(\mathbb{R}_+) : f'(0) = 0\}$. If, in addition $q \in L^1(\mathbb{R}_+)$, then $\sigma_{ac}(H_{X,\alpha,q}) = \mathbb{R}_+$.

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Thank for your attention!