Schrödinger operators with singular interactions on a non-discrete set

Edison Leguizamón

Universidad de los Andes

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The Schrödinger equation

The possible states that the electron can occupy are determined by the Schrödinger equation

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We study the differential expression

$$\mathcal{H}:=-\frac{d^2}{dx^2}+V(x),\quad \text{on } (a,b).$$

- $V \in L^1_{\text{loc}}(a,b)$ and real ☺
- V is a distribution ☹
- V is complex ☹

Konnig-Penney Model

Quantum Mechanics of Electrons in Crystal Lattices.

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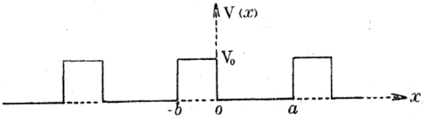

Figure: Potential

- $b \to 0$ and $V_0 \to \infty$.

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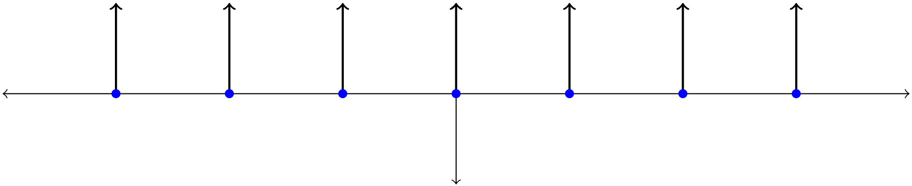
$$V(x) \approx \sum \delta(x - na)$$



"The energy values which an electron moving through the lattice may have, hence form a spectrum consisting of continuous pieces separated by finite intervals." Kronig-Penney 1930.

Schrödinger equation with δ interactions

- $X = (x_n)$, $\alpha = (\alpha_n) \subset \mathbb{R}$ with (x_n) increasing.

The energy states are determined by the equation

$$-\frac{d^2 f}{dx^2} + \sum_{n=1}^{\infty} \alpha_n \delta(x - x_n) f = Ef.$$

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We want to study the differential expression

$$\mathcal{U} f := -\frac{d^2 f}{dx^2} + q(x) f + \sum_{n=1}^{\infty} \alpha_n \delta(x - x_n) f. \qquad (\mathcal{U})$$

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Is it possible to find a self-adjoint operator for this differential expression?

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Weyl-Titchmarsh function

Consider the Sturm-Liouville problem

$$-y''(x) + V(x)y(x) = \lambda y(x), \quad x \in [a, b).$$

Let $\{$u,v$\}$ be a fundamental system with boundary conditions

$$u(a, \lambda) = 0, \quad v(a, \lambda) = 1,$$
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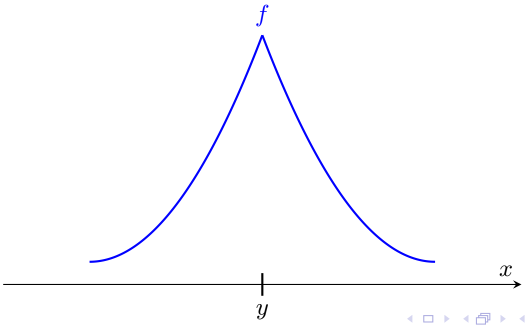

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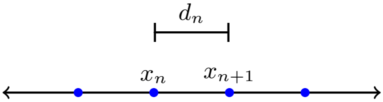

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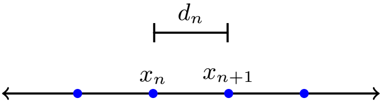

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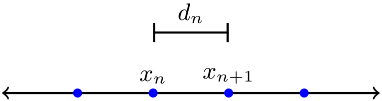

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Is A_α always self-adjoint? What about $\sigma(A_\alpha)$?

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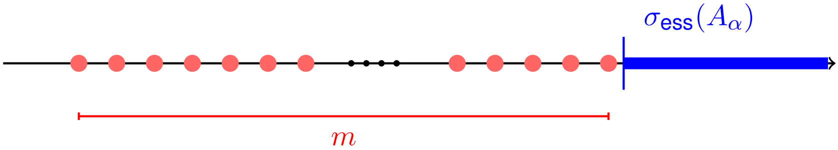

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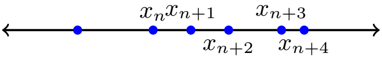

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- If $\lim_{n\to\infty} \alpha_n d_n^{-1} = \infty$, then

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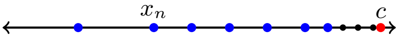

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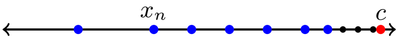

- (Eckhardt, Teschl 2014) If $\alpha \in l^1(\mathbb{R})$,

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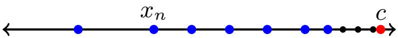

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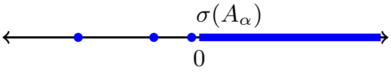

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- Can embedded eigenvalues appear in the essential spectrum of A_α?

In (Eckhart and Teschl, 2013) they introduce measure valued Sturm-Liouville problems.

Quasi-derivative

Let μ be a locally finite Borel complex measure. A μ-measurable function f is called absolutely continuous with respect to μ if there exists a measurable function h such that

$$f(x) = f(c) + \int_c^x h \, d\mu, \quad \text{for all } x, c \in \mathbb{R}.$$

We say that h is the quasi-derivative of f and we denote it by $\frac{df}{d\mu}$.

Linear measure differential equations

Let μ, χ be complex Borel measures. Consider the differential expression on $\mathbb{R}$

$$\tau f := -\frac{d}{dx}\left(\frac{df}{d\mu} + \int_c^x f \, d\chi\right). \tag{τ}$$

Here $\frac{d}{dx}$ represents the derivative with respect to the Lebesgue measure.

Singular interactions as measures

δ-interactions

- If $\mu = \lambda$, and $\chi = \sum_{n=1}^{\infty} \alpha_n \delta_{x_n}$, then (τ) coincides with $(\mathcal{U})$.
- Conditions: $f^{[1]}(x_n+) - f^{[1]}(x_n-) = \alpha_n f(x_n)$.

Theorem (Eckhart,Teschl 2013)

- *There exists a Weyl function as in the classical case and the poles of $m(\cdot)$ are the eigenvalues of A_α.*

Fundamental system

Proposition (Leguizamón, Winklmeier, 2024)

The fundamental system for (τ) *is* $\{u(\cdot,\lambda), v(\cdot,\lambda)\}$*, given by*

$$u(x,\lambda) = \frac{-1}{\sqrt{\lambda}} \sum_{n\in\mathbb{N}} \alpha_n u_n H(x-x_n)\left(\sin(\sqrt{\lambda}(x-x_n))\right) + \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}},$$

$$v(x,\lambda) = \frac{-1}{\sqrt{\lambda}} \sum_{n\in\mathbb{N}} \alpha_n v_n H(x-x_n)\left(\sin(\sqrt{\lambda}(x-x_n))\right) + \cos(\sqrt{\lambda}x),$$

where $H(\cdot)$ *is the Heaviside function and*

$$u_n = \frac{\sin(\sqrt{\lambda}\,x_n)}{\sqrt{\lambda}} - \frac{1}{\sqrt{\lambda}} \sum_{j<n} \alpha_j u_j \sin(\sqrt{\lambda}(x_n - x_j)),$$

$$v_n = \cos(\sqrt{\lambda}\,x_n) - \frac{1}{\sqrt{\lambda}} \sum_{j<n} \alpha_j v_j \sin(\sqrt{\lambda}(x_n - x_j)).$$

Formula for the eigenvalues

Proposition (Leguizamón, Winklmeier, 2024)

The Weyl function of A_α is

$$m(\lambda) = -\left(\frac{\frac{1}{i\sqrt{\lambda}} \sum_{n\in\mathbb{N}} \alpha_n v_n e^{i\sqrt{\lambda}\, x_n} + 1}{\frac{1}{i\sqrt{\lambda}} \sum_{n\in\mathbb{N}} \alpha_n u_n e^{i\sqrt{\lambda}\, x_n} - \frac{1}{i\sqrt{\lambda}}} \right).$$

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- We have analogous results for δ' interactions.

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¡Gracias!