On the spectrum of the Kronig–Penney model in a constant electric field

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joint work with
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Djurö, August 2021

The problem

Consider the one-dimensional Schrödinger operator

$$L_{F,\lambda} = -\frac{d^2}{dx^2} - Fx + \lambda \sum_{n\in\mathbb{Z}} \delta(x-n) \quad \text{in } L^2(\mathbb{R})$$

with $F, \lambda \in \mathbb{R}$.

Question: How do spectral properties of $L_{F,\lambda}$ depend on the parameters?

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Some special cases:

- $F = 0$, $\lambda = 0$ then $\sigma = [0, \infty)$ only ac (the Laplace operator)
- $F \neq 0$, $\lambda = 0$ then $\sigma = \mathbb{R}$ only ac (the Stark operator),
- $F = 0$, $\lambda \neq 0$ then spectrum is only ac with band structure (the Kronig–Penney model)

In general case few **mathematically rigorous** results exist.

Ao '90, and independently Buslaev '99, suggested that the nature of the spectrum depends on number theoretic properties of F and the size of F/λ^2.

In Berezhkovskii–Ovchinnikov '76 and Borysowicz '97 the potential for number theoretic dependence is missed.

Main results

$$L_{F,\lambda} = -\frac{d^2}{dx^2} - Fx + \lambda \sum_{n\in\mathbb{Z}} \delta(x-n) \text{ with } F > 0 \text{ and } \lambda \in \mathbb{R}$$

Theorem (Frank–L., '21)

Fix $F \in \pi^2\mathbb{Q}_+, \lambda \in \mathbb{R}$ and write $F = \frac{\pi^2}{3}\frac{p}{q}$ with $p, q \in \mathbb{N}$. Then

$$\sigma_{ac}(L_{F,\lambda}) = \mathbb{R}\,, \qquad \sigma_{sc}(L_{F,\lambda}) = \emptyset\,, \qquad \sigma_{pp}(L_{F,\lambda}) \subseteq \left\{\frac{\pi^2}{3q}m + \lambda : m \in \mathbb{Z}\right\}.$$

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Remarks:

- By translation by 1 the spectrum of $L_{F,\lambda}$ is F periodic so the possible eigenvalues only depend on m through $m \mod p$.
- The δ is a critical case. If $L = -\frac{d^2}{dx^2} - Fx + V$ then
  - $V \in L^1 \cap H^{-1/2}(\mathbb{R}/\mathbb{Z}) \implies \sigma_{ac}(L) = \mathbb{R}$ (Galina Perelman '03)
  - $V = \sum \delta'(x-n) \implies \sigma_{ac}(L) = \emptyset$ (Avron–Exner–Last '94, Exner '95)
- We push techniques used by Perelman '05 to prove related results.
- While the theorem assumes $F \in \pi^2\mathbb{Q}_+$ most of our work does not need this assumption.
- When $F \in \mathbb{R}_+ \setminus \pi^2\mathbb{Q}_+$ one expects a transition from singular continuous to pure point spectrum as λ^2/F is increased.

Main results

$L^{\omega}_{F,\lambda} = -\frac{d^2}{dx^2} - Fx + \sum_{n\in\mathbb{Z}} g_n(\omega)\delta(x-n)$, with $F > 0$ and $g_n(\omega)$ independent random variables, at least one having ac distribution and for all n

$$\mathbb{E}_\omega[g_n] = 0\,, \quad \mathbb{E}_\omega[g_n^2] = \lambda^2\,, \quad \mathbb{E}_\omega[|g_n|^\beta] < C \quad \text{for some } \beta > 4.$$

Theorem (Frank–L., '21)

Almost surely $L^{\omega}_{F,\lambda}$ defines a self-adjoint operator in $L^2(\mathbb{R})$ with $\sigma(L^{\omega}_{F,\lambda}) = \mathbb{R}$. Moreover, the spectrum is almost surely

- *purely singular continuous if $F > \lambda^2/2$,*
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Remarks:

- Delyon–Simon–Souillard '85 proved $\begin{cases} F/\lambda^2 \text{ small} \implies \text{a.s. only pp} \\ F/\lambda^2 \text{ large} \implies \text{a.s. continuous spectrum} \end{cases}$
- For $-\frac{d^2}{dx^2} - Fx + \lambda W_\omega$ (W_ω white noise) analogue result by Minami '92
- Kiselev–Last–Simon '97 considered $-\Delta + \frac{g_n(\omega)}{(1+|n|)^\alpha}$ in $l^2(\mathbb{Z})$, analogue result in critical case $\alpha = 1/2$.
- If $F > \lambda^2/2$, a.s. spectral measure vanishes on sets of Hausdorff dim. less than $1 - \frac{\lambda^2}{2F}$ (by techniques of Jitomirskaya–Last '99 & '00 and Damanik–Killip–Lenz '00).

Reduction to ODE's

By Gilbert–Pearson subordinacy theory and in the random case the theory of rank-one perturbations (spectral averaging) proof is reduced to analysing solutions of the ODE

$$-\psi''(x) - Fx\psi(x) = E\psi(x) \quad \text{in } \mathbb{R} \setminus \mathbb{Z}$$
$$J\psi(n) = 0 \quad \text{and} \quad J\psi'(n) = g_n\psi(n) \quad \text{for } n \in \mathbb{Z}\,.$$

where $Ju(x) = \lim_{\varepsilon \to 0^+} \big[u(x+\varepsilon) - u(x-\varepsilon)\big]$ and $g_n = \lambda$ or $g_n = g_n(\omega)$.

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Specifically:

1. Does there exist a solution of the equation subordinate at $\pm\infty$?
2. If they exist, are the subordinate solutions square integrable?

Definition A non-trivial solution ψ is subordinate at $+\infty$ if for any lin. indep. solution η

$$\lim_{M\to\infty}\frac{\int_0^M |\psi(x)|^2\,dx}{\int_0^M |\eta(x)|^2\,dx} = 0\,.$$

Subordinacy at $-\infty$ is defined similarly.

Main ODE results

Lemma (Both models)

For all $E \in \mathbb{R}$ there exists a solution ψ of the eigenvalue equation subordinate and square integrable at $-\infty$.

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Proposition (Deterministic model)

For $F \in \pi^2\mathbb{Q}_+$, $F = \frac{\pi^2}{3}\frac{q}{p}$, and $E \in \mathbb{R} \setminus \{\frac{\pi^2}{3p}m + \lambda : m \in \mathbb{Z}\}$ there exists no solution of the eigenvalue equation subordinate at $+\infty$.

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Proposition (Random model)

Let $F > 0$, $E \in \mathbb{R}$ and g_n be independent r.v.'s as before. Then

i) *for every boundary condition at 0 the corresponding solution ψ of the eigenvalue equation satisfies, almost surely,*

$$\int_M^{M+1} |\psi(x)|^2 \, dx = M^{-\frac{1}{2}+\frac{\lambda^2}{4F}+o(1)} \quad \text{as } M \to \infty \, .$$

ii) *almost surely there exists a boundary condition at 0 such that the corresponding solution ψ of the eigenvalue equation satisfies*

$$\int_M^{M+1} |\psi(x)|^2 \, dx = M^{-\frac{1}{2}-\frac{\lambda^2}{4F}+o(1)} \quad \text{as } M \to \infty \, .$$

Relative Prüfer coordinates

Define the reference solution

$$\zeta(x) = \left(\frac{\pi}{F^{1/3}}\right)^{1/2}\Big(i\mathrm{Ai}(-F^{1/3}(x+E/F)) + \mathrm{Bi}(-F^{1/3}(x+E/F))\Big)$$

which satisfies

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Lemma

There exists real-valued and increasing $\gamma \in C^\infty(\mathbb{R})$ such that

$$\zeta(x) = \frac{e^{i\gamma(x)}}{\sqrt{\gamma'(x)}}\,,$$

$$\gamma(x) = \frac{2\sqrt{F}}{3}x^{3/2} + \frac{E}{\sqrt{F}}x^{1/2} + \frac{\pi}{2} + O(x^{-1/2})\,,$$

and the asymptotic expansion can be differentiated.

Relative Prüfer coordinates, complex set-up

Let ψ be a **real-valued** solution of the eigenvalue equation then there exists uniquely determined $\{\alpha(n)\}_{n\in\mathbb{Z}} \subset \mathbb{C} \setminus \{0\}$ such that

$$\psi(x) = \alpha(n)\zeta(x) + \overline{\alpha}(n)\overline{\zeta}(x) \quad \text{for } x \in (n-1, n]\,.$$

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Lemma

Set $U(n) = \frac{g_n}{\gamma'(n)}$, *then*

$$\begin{pmatrix}\alpha(n+1)\\ \overline{\alpha}(n+1)\end{pmatrix} = A_n \begin{pmatrix}\alpha(n)\\ \overline{\alpha}(n)\end{pmatrix} \quad \textit{with } A_n = \mathbb{1} + \frac{U(n)}{2i}\begin{pmatrix}1 & e^{-2i\gamma(n)}\\ -e^{2i\gamma(n)} & -1\end{pmatrix}.$$

Furthermore,

$$\int_{n-1}^{n} |\psi(x)|^2\,dx \sim \frac{|\alpha(n)|^2}{n^{1/2}}\,.$$

Remarks:

1) Same structure as equations appearing for OPUC, $A_n \in \mathbb{SU}(1,1)$.
2) The non-linear phase γ differs from more classical case.
3) $U(n) \sim n^{-1/2}$ matches critical decay rate in Kiselev–Last–Simon '97.

Relative Prüfer coordinates

Define the Prüfer Radius and angle $R, \eta \colon \mathbb{N} \to \mathbb{R}$ by

$$\alpha(n) = \frac{R(n)}{2i} e^{i\eta(n)} \quad \text{and let} \quad \theta(n) = \gamma(n) + \eta(n)\,,$$

with $\eta(1) \in (-\pi, \pi]$ and $\eta(n+1) - \eta(n) \in (-\pi, \pi]$.

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Then

$$R(n+1)^2 = R(n)^2 \Big[1 + U(n) \sin(2\theta(n)) + U(n)^2 \sin^2(\theta(n)) \Big]\,,$$

$$\cot(\eta(n+1) + \gamma(n)) = \cot(\eta(n) + \gamma(n)) + U(n)\,.$$

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Since $U(n) = \frac{g_n}{\gamma'(n)} \sim n^{-1/2} \to 0$ (almost surely),

$$\log\Big(\frac{R(n+1)}{R(n)}\Big) = \frac{U(n)}{2}\sin(2\theta(n)) + \frac{U(n)^2}{8} + \frac{U(n)^2}{8}\Big[\cos(4\theta(n)) - \frac{1}{2}\cos(2\theta(n))\Big] + O(|U(n)|^3)$$

Repeated use of the equations yield

$$\log\Big(\frac{R(N+1)}{R(1)}\Big) = \frac{1}{2}\sum_{n=1}^{N} U(n)\sin(2\theta(n)) + \frac{1}{8}\sum_{n=1}^{N} U(n)^2 + \frac{1}{8}\sum_{n=1}^{N} U(n)^2\Big[\cos(4\theta(n)) - \frac{1}{2}\cos(2\theta(n))\Big] + O(1)$$

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Need to understand exponential sums of the form

$$\sum_{a<n\le b}\Big(\frac{g_n}{\gamma'(n)}\Big)^m e^{i\mu\theta(n)} \quad \text{with} \begin{cases} m = 1, 2\,, \\ \mu = 2, 4\,, \\ g_n \equiv \lambda \text{ or } g_n \text{ indep. r.v.'s} \end{cases}$$

Heuristically: $\theta = \gamma + \eta$ can be treated as a small perturbation of γ.

The random model

$g_n(\omega)$ indep. r.v.'s with $\mathbb{E}_\omega[g_n] = 0$, $\mathbb{E}_\omega[g_n^2] = \lambda^2$.

Claim: for any $R(1), \eta(1)$ almost surely

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Remarks:

- Abstract $\mathbb{SU}(1,1)$ machinery implies existence of subordinate solution.
- Only the last estimate does not work for deterministic model.

The deterministic model

Problem: In general we are not able to accurately compute asymptotics of

$$\sum_{n=1}^{N} \frac{e^{i2\gamma(n)}}{\gamma'(n)} \quad \text{as } N \to \infty.$$

Recall: $\gamma(x) = \frac{2\sqrt{F}}{3}x^{3/2} + \frac{E}{\sqrt{F}}x^{1/2} + \frac{\pi}{2} + O(x^{-1/2})\,.$

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However we can understand partial sums of lengths larger than $O(1)$

$\implies$ we can coarse grain our equations.

- Strong cancellations unless $\gamma'(x)$ close to $\pi\mathbb{Z}$.
- Define X_l by $\gamma'(X_l) = \pi l$,

$$\gamma'(x) = \sqrt{F} x^{1/2} + O(x^{-1/2}) \quad \implies \quad X_l = \frac{\pi^2}{F} l^2 + O(1),$$

  natural scale is given by $x \sim \frac{\pi^2}{F} l^2$.
- By combination of Poisson summation formula and the method of stationary phase we can accurately compute

$$\sum_{n \in I_l} \frac{e^{2i\gamma(n)}}{\gamma'(n)} \quad \text{with } I_l = \left(\tfrac{\pi^2}{F} \left(l - \tfrac{1}{2}\right)^2, \tfrac{\pi^2}{F} \left(l + \tfrac{1}{2}\right)^2 \right].$$

Theorem (Frank–L., '21)

Fix $F > 0, E \in \mathbb{R}, \lambda \in \mathbb{R}$, *and set* $I_l = \big(\frac{\pi^2}{F}(l-\frac{1}{2})^2,\ \frac{\pi^2}{F}(l+\frac{1}{2})^2\big]$.
Let ψ *be a real-valued solution of the eigenvalue equation, then there exist* $\mathcal{R}, \Lambda\colon \mathbb{N} \to \mathbb{R}$ *such that for* $x \in I_l$

$$\psi(x) = \mathcal{R}(l)\frac{e^{i\Lambda(l)-i\lambda\sqrt{\lceil x\rceil/F}}\zeta(x) - e^{-i\Lambda(l)+i\lambda\sqrt{\lceil x\rceil/F}}\overline{\zeta}(x)}{2i} + O\Big(\frac{\mathcal{R}(l)|\zeta(x)|}{\sqrt{l}}\Big).$$

Moreover, $\mathcal{R}, \Lambda$ *satisfy*

$$\log\Big(\frac{\mathcal{R}(l+1)}{\mathcal{R}(l)}\Big) = \frac{\lambda\sin(2\Theta(l))}{\sqrt{2Fl}} + \frac{\lambda^2}{4Fl}\Big[1+\cos(4\Theta(l))\Big] + O(l^{-5/4}),$$

$$\Lambda(l+1) - \Lambda(l) = \frac{\lambda\cos(2\Theta(l))}{\sqrt{2Fl}} + O(l^{-3/4}),$$

where

$$\Theta(l) = \Gamma(l) + \Lambda(l) \qquad \text{and} \qquad \Gamma(l) = -\frac{\pi^3}{3F}l^3 + \frac{\pi}{F}(E-\lambda)l + \frac{5\pi}{8},$$

Remarks:

- $|\zeta(x)| \sim l^{-1/2}$ on I_l.
- Main term in representation of ψ solves equation between integers.
- Higher order terms in Λ equation are known but complicated.

The deterministic model, the rational case

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Write $F = \frac{\pi^2}{3}\frac{p}{q}$ and compute change of $\mathcal{R}, \Lambda$ when from $l = pk$ to $l = p(k+1)$.

$$\sum_{l=pk}^{p(k+1)-1} \frac{e^{2i\Gamma(l)+2i\Lambda(l)}}{\sqrt{l}} \approx \frac{e^{2i\Gamma(pk)+2i\Lambda(pk)}}{\sqrt{pk}} \sum_{j=0}^{p-1} e^{2i(\Gamma(pk+j)-\Gamma(pk))}$$

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Key observation: For $k \in \mathbb{N}$, $j = 0, \dots, p-1$,

$$\Gamma(pk) = \underbrace{-\pi q p^2 k^3}_{\in \pi\mathbb{Z}} + \underbrace{\frac{\pi p}{F}(E-\lambda)k + \frac{5\pi}{8}}_{\text{linear!}}$$

$$\Gamma(pk+j) - \Gamma(pk) = \underbrace{-3\pi q k j^2 - 3pqk^2 j}_{\in \pi\mathbb{Z}} \underbrace{-\frac{\pi q}{p} j^3 + \frac{\pi}{F}(E-\lambda)j}_{\text{independent of } k}$$

$\Longrightarrow$ A new effective problem with linear phase!

Summary and conclusion

We considered

$$-\frac{d^2}{dx^2} - Fx + \sum_{n\in\mathbb{Z}} g_n\delta(x-n) \quad \text{in } L^2(\mathbb{R})\,.$$

- For $g_n \equiv \lambda$ and $F \in \pi^2\mathbb{Q}$ we prove that the spectrum is pure ac away from an explicit set of possible eigenvalues.
- For g_n independent random variables with $\mathbb{E}[g_n] = 0, \mathbb{E}[g_n^2] = \lambda^2$ we prove transition from pp to sc spectrum as F/λ^2 increases.
- Using relative Prüfer coordinates the problem is reduced to a discrete system resembling the OPUC setting which is analysed using exponential sum estimates.
- It remains an open problem what happens when $F \notin \pi^2\mathbb{Q}$ in first model and when $F/\lambda^2 = 1/2$ in second.

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Thank you for your attention!