On the Kronig–Penney model in a constant electric field

Simon Larson
Chalmers University of Technology &
The University of Gothenburg

joint work with R. L. Frank

Mathematical results of many-body quantum systems
Herrsching, June 2022

The problem

Consider the one-dimensional Schrödinger operator

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

with $F \in \mathbb{R}$, $a > 0$, and $g = \{g_n\}_{n\in\mathbb{Z}} \subset \mathbb{R}$.

We shall look at two particular cases:

Model I: $g_n \equiv \lambda \in \mathbb{R}$.

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

Question: How do spectral properties of these operators depend on the parameters F, a, and λ?

Q1: Is the spectrum discrete, p.p., s.c., a.c., or a combination thereof?

Q2: How do solutions of the eigenvalue equation decay/grow at $\pm\infty$?

Some background – Model I

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

The Hamiltonian arises in two different physical settings

1. a periodic crystal in a **constant electric field**,
2. a conducting ring with a point-like defect threaded by a **magnetic flux** which increases linearly in time.

Its properties was a topic of discussion in solid state physics during the 80's.

When $F, \lambda \neq 0$ few **mathematically rigorous** results exist.

Berezhkovskii–Ovchinnikov '76 and Borysowicz '97 argued that $\sigma(L_{F,\lambda,a}) = \mathbb{R}$ and only p.p. or s.c. depending only on the size of $\lambda^2/(aF)$.

Ao '90, and independently Buslaev '99, suggested that the nature of the spectrum also depends on number-theoretic properties of a^3F.

Some background – Model II

$$L^{\omega}_{F,\lambda,a} = -\frac{d^2}{dx^2} - Fx + \sum_{n\in\mathbb{Z}} g_n(\omega)\delta(x-an), \qquad F > 0$$

Studied (numerically) by Soukoulis et al. '83 and later by Delyon, Simon, Souillard '84 and '85.

Drastically different behavior than for disordered systems with $F = 0$ and/or if the disordered potential is replaced by something more regular.

Specifically Delyon–Simon–Souillard '85 proved that almost surely $\sigma(L^{\omega}_{F,\lambda,a}) = \mathbb{R}$ and

- if $\frac{\lambda^2}{aF}$ is **small** then the spectrum is purely continuous, and
- if $\frac{\lambda^2}{aF}$ is **large** then the spectrum is pure point spectrum with eigenfunctions decaying as $x^{-\beta(F,\lambda,a)}$ when $x \to +\infty$.

If the disordered potential is replaced by white noise such behavior was predicted by Prigodin '80 and confirmed in Minami '92.

Main results

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

Theorem (Frank–L., '21)

Fix $F, a > 0$ and $\lambda \in \mathbb{R}$ such that $a^3F \in \pi^2\mathbb{Q}_+$ and write $a^3F = \frac{\pi^2 p}{q}$ with $p, q \in \mathbb{N}$. Then

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

Remarks:

- Contradicts the predictions of Berezhkovskii–Ovchinnikov and Borysowicz and partially confirms those of Ao and Buslaev.
- By translation by a the spectrum of $L_{F,\lambda,a}$ is aF periodic so the possible eigenvalues only depend on m through $m \mod q$.
- The δ is a critical case. If $L = -\frac{d^2}{dx^2} - Fx + V$ then
  - $V \in L^1 \cap H^{-1/2}(\mathbb{R}/(a\mathbb{Z})) \implies \sigma_{ac}(L) = \mathbb{R}$ (Galina Perelman '03)
  - $V = \sum \delta'(x-an) \implies \sigma_{ac}(L) = \emptyset$ (Avron–Exner–Last '94, Exner '95)

Main results

$L^{\omega}_{F,\lambda} = -\frac{d^2}{dx^2} - Fx + \sum_{n\in\mathbb{Z}} g_n(\omega)\delta(x-an)$, 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 $L^{\omega}_{F,\lambda,a}$ defines a self-adjoint operator in $L^2(\mathbb{R})$ with $\sigma(L^{\omega}_{F,\lambda,a}) = \mathbb{R}$. Moreover, the spectrum is almost surely

- *purely singular continuous if $\frac{\lambda^2}{aF} < 2$,*
- *only pure point if $\frac{\lambda^2}{aF} > 2$.*

Remarks:

- Improves the result of Delyon–Simon–Souillard '85.
- For $-\frac{d^2}{dx^2} - Fx + \lambda W_\omega$ in $L^2(\mathbb{R}_+)$ the analogue result was obtained by Minami '92 (confirming Prigodin's prediction).
- Kiselev–Last–Simon '97 proved an analogue for $-\Delta + \frac{g_n(\omega)}{(1+|n|)^{1/2}}$ in $l^2(\mathbb{Z})$.

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

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

where

$$Ju(x) = \lim_{\varepsilon \to 0^+} \big[u(x+\varepsilon) - u(x-\varepsilon)\big].$$

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.

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

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

where

$$Ju(x) = \lim_{\varepsilon \to 0^+} \big[u(x+\varepsilon) - u(x-\varepsilon)\big].$$

Specifically:

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

Gilbert–Pearson theory:

$$\begin{aligned}\{E \in \mathbb{R} : \exists \text{sol. } \psi \in L^2(\mathbb{R})\} &= \text{point spectrum} \\ \{E \in \mathbb{R} : \exists \text{sol. } \psi \notin L^2(\mathbb{R}) \text{ subord. at both } \pm\infty\} &\sim \text{s.c. spectrum} \\ \{E \in \mathbb{R} : \exists \text{direction in which no sol. } \psi \text{ is subord.}\} &\sim \text{a.c. spectrum}\end{aligned}$$

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 $-\infty$.

Proposition (Deterministic model)

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

Proposition (Random model)

Let $F, a > 0$, $E \in \mathbb{R}$ and g_n be independent r.v.'s as before. Then almost surely there exist linearly independent solutions $\psi_\pm$ of the eigenvalue equation satisfying

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

In particular, ψ_- is subordinate at $+\infty$.

Relative Prüfer coordinates

There exists a function ζ, which we call the reference solution, satisfying

$$-\zeta''(x) - Fx\zeta(x) = E\zeta(x) \quad \text{and} \quad \{\zeta, \bar{\zeta}\}(x) \neq 0.$$

Lemma

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

$$\zeta(x) = F^{1/6} \frac{e^{i\gamma(x)}}{\sqrt{\gamma'(x)}}\,,$$

$$\gamma(x) = \frac{2\sqrt{Fx^3}}{3} + O(x^{1/2})\,,$$

and the asymptotic expansion can be differentiated.

Relative Prüfer coordinates

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

$$\psi(x) = \alpha(n)\zeta(x) + \beta(n)\overline{\zeta}(x) \quad \text{for } a(n-1) < x \leq an\,.$$

Lemma

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

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

Furthermore,

$$\int_{a(n-1)}^{an} |\psi(x)|^2\, dx \sim \frac{|\alpha(n)|^2 + |\beta(n)|^2}{\sqrt{n}}\,.$$

Aim: We want to understand behavior of the products $A_N \cdots A_1$ as $N \to \infty$.

Relative Prüfer coordinates

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

$$\psi(x) = \alpha(n)\zeta(x) + \beta(n)\overline{\zeta}(x) \quad \text{for } a(n-1) < x \leq an\,.$$

Lemma

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

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

Furthermore,

$$\int_{a(n-1)}^{an} |\psi(x)|^2\, dx \sim \frac{|\alpha(n)|^2 + |\beta(n)|^2}{\sqrt{n}}\,.$$

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) Random model closely related to one studied in Kiselev–Last–Simon '97.

Relative Prüfer coordinates

Assume that ψ is **real-valued**.

Then $\beta(n) = \overline{\alpha(n)}$ and we define the Prüfer Radius and angle $R, \eta\colon \mathbb{N} \to \mathbb{R}$ by

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

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

Lemma

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

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

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

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

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

Repeated use of the equations yield

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

$$
\begin{aligned}
\eta(N+1) - \eta(1) &= -\frac{1}{2}\sum_{n=1}^{N} U(n) + \frac{1}{2}\sum_{n=1}^{N} U(n)\cos(2\theta(n)) \\
&\quad + \frac{1}{8}\sum_{n=1}^{N} U(n)^2\Big[2\sin(2\theta(n)) - \sin(4\theta(n))\Big] + O(1)
\end{aligned}
$$

We are left with trying to understand exponential sums of the form

$$
\sum_{n_1<n\leq n_2} \Big(\frac{g_n}{\gamma'(an)}\Big)^m e^{i\mu\theta(n)} \quad \text{with} \begin{cases} m = 1, 2\,, \\ \mu = 2, 4\,, \\ g_n \equiv \lambda \text{ or } g_n \text{ indep. r.v.'s} \end{cases}
$$

- We aim to treat $\theta = \gamma + \eta$ as a 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

$$\log\Big(\frac{R(N+1)}{R(1)}\Big) = \frac{\lambda^2}{8aF}\log(N)(1+o(1)).$$

Proof follows closely Kiselev–Last–Simon '97 using Martingale bounds and van der Corput-type estimate.

This corresponds to that almost surely

$$\|A_N^\omega \cdots A_1^\omega\| = N^{\frac{\lambda^2}{4aF}+o(1)} \quad \text{as } N \to \infty$$

where as before

$$A_n^\omega = \mathbb{1} + \frac{U(n)}{2i}\begin{pmatrix} 1 & e^{-2i\gamma(an)} \\ -e^{2i\gamma(an)} & -1 \end{pmatrix}.$$

Or that for fixed boundary condition at zero the corresponding solution of our eigenvalue equation almost surely satisfies

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

The deterministic model

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

$$\sum_{n=1}^{N} \frac{\lambda e^{2i\gamma(an)+2i\eta(n)}}{\gamma'(an)} \quad \text{as } N \to \infty.$$

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

$\implies$ we can coarse grain our equations.

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

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

  $$a\gamma'(an) = \sqrt{a^3F}n^{1/2} + O(n^{-1/2}) \quad \implies \quad X_l = \frac{\pi^2}{a^3F}l^2 + O(1),$$

  natural scale is given by $n \sim \frac{\pi^2}{a^3F}l^2$ (or equivalently $x \sim \frac{\pi^2}{a^2F}l^2$).
- By combining Poisson summation formula and the method of stationary phase we can accurately compute

  $$\sum_{n\in I_l} \frac{\lambda e^{2i\gamma(an)}}{\gamma'(an)} \quad \text{with } I_l = \left(\tfrac{\pi^2}{a^3F}\left(l-\tfrac{1}{2}\right)^2, \tfrac{\pi^2}{a^3F}\left(l+\tfrac{1}{2}\right)^2\right].$$

Theorem (Frank–L., '21)

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* $x \in \left(\frac{\pi^2}{a^2F}(l-\frac{1}{2})^2,\ \frac{\pi^2}{a^2F}(l+\frac{1}{2})^2\right]$

$$\psi(x) = \Im\Big[\mathcal{R}(l)\zeta(x)e^{i\Lambda(l)-i\lambda\sqrt{\lceil x/a\rceil/(aF)}}\Big] + O\Big(\frac{\mathcal{R}(l)|\zeta(x)|}{\sqrt{l}}\Big).$$

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

$$\log\Big(\frac{\mathcal{R}(l+1)}{\mathcal{R}(l)}\Big) = \frac{\lambda\sin(2\Theta(l))}{\sqrt{2aFl}} + \frac{\lambda^2}{4aFl}\Big[1+\cos(4\Theta(l))\Big] + O(l^{-5/4}),$$
$$\Lambda(l+1)-\Lambda(l) = \frac{\lambda\cos(2\Theta(l))}{\sqrt{2aFl}} + O(l^{-3/4}),$$

where

$$\Theta(l) = \Gamma(l)+\Lambda(l) \qquad \text{and} \qquad \Gamma(l) = -\frac{\pi^3}{3a^3F}l^3 + \frac{\pi}{a^3F}(a^2E-a\lambda)l + \frac{5\pi}{8},$$

Remarks:

- Does not assume $a^3F \in \pi^2\mathbb{Q}$.
- Started with $\psi(x) = \Im[R(n)e^{i\eta(n)}\zeta(x)]$ on $(a(n-1), an)$, the result is an approximate analogue on the growing intervals I_l ($|I_l| \sim l/(a^2F)$).
- Implies that $\sigma(L_{F,\lambda,a}) = \mathbb{R}$ for all $F, a > 0, \lambda \in \mathbb{R}$.

Theorem (Frank–L., '21)

Set $I_l = \big(\frac{\pi^2}{a^3F}(l-\frac12)^2,\ \frac{\pi^2}{a^3F}(l+\frac12)^2\big]$.
Then

$$\prod_{n\in I_l\cap\mathbb{Z}} A_n = A_{\lfloor \frac{\pi^2}{F}(l+\frac12)^2\rfloor}\cdots A_{\lceil \frac{\pi^2}{F}(l-\frac12)^2\rceil} = U(l+1)T(l)U(l)^{-1}$$

where $T, U \in \mathbb{SU}(1,1)$ *are explicit. In particular,*

$$T(l) = \begin{pmatrix} 1+\frac{\lambda^2}{4aFl} & -\frac{i\lambda e^{-2i\Gamma(l)}}{\sqrt{2aFl}} \\ \frac{i\lambda e^{2i\Gamma(l)}}{\sqrt{2aFl}} & 1+\frac{\lambda^2}{4aFl}\end{pmatrix} + O(l^{-5/4})$$

with

$$\Gamma(l) = -\frac{\pi^3}{3a^3F}l^3 + \frac{\pi}{a^3F}(a^2E - a\lambda)l + \frac{5\pi}{8}\,,$$

Note: Improved growth estimate for the norm of transfer matrices,

$$\|A_N\cdots A_1\| \le \prod_{n=1}^N \|A_n\| \approx \prod_{n=1}^N\Big(1+\frac{|\lambda|}{\sqrt{aFn}}\Big) \approx e^{c\sqrt{N}}$$

$$\|A_N\cdots A_1\| \le \prod_{l=1}^{\sqrt{a^3FN}} \|T(l)\| \approx \prod_{l=1}^{\sqrt{a^3FN}}\Big(1+\frac{|\lambda|}{\sqrt{2aFl}}\Big) \approx e^{\tilde{c}N^{1/4}}.$$

The deterministic model – the rational case

Question: What makes $a^3F \in \pi^2\mathbb{Q}$ special?

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

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

Observation: Since $\Gamma(l) = -\frac{\pi^3}{3a^3F}l^3 + \frac{\pi}{a^3F}(a^2E - a\lambda)l + \frac{5\pi}{8}$ for all $k, j \in \mathbb{N}$

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

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

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

Thank you for your attention!