Periodic quantum graphs may exhibit uncommon spectra

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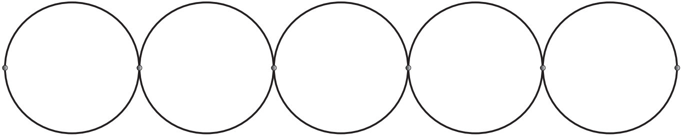
Only wimps specialize in the general case. Real scientists pursue examples.

First example: chain graphs

Consider a *chain graph*, an array of identical rings as sketched here



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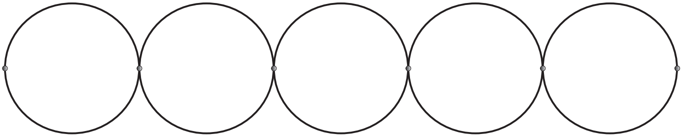

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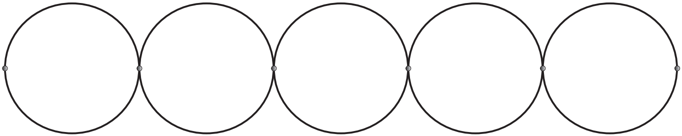

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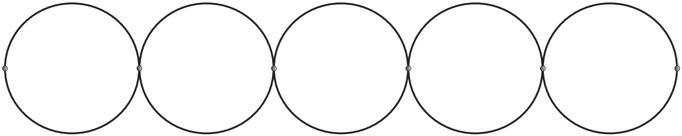

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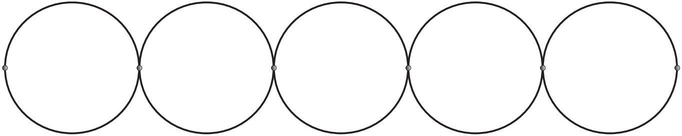

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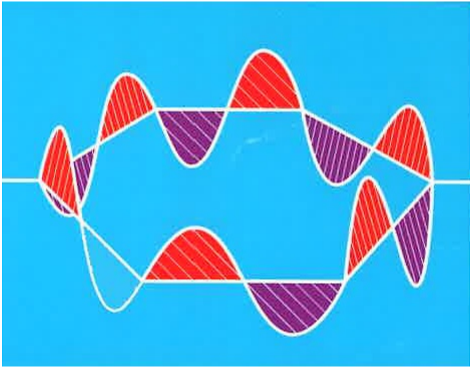
Hence the spectrum is not purely *ac* and this trivial conclusion remains valid even if the chain loses it s mirror symmetry but the 'upper' and 'lower' edge lengths are *rationally related*

Dirichlet eigenvalues are easy to understand

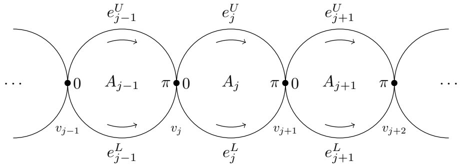


Courtesy: Peter Kuchment

It is also clear that quantum graphs can have compactly supported eigenfunctions

Spectrum may not be absolutely continuous at all

To illustrate this less trivial claim, consider the same graph exposed to a magnetic field as sketched below



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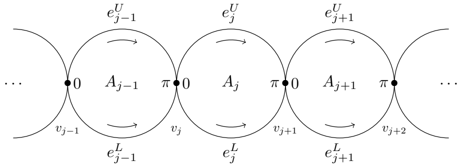

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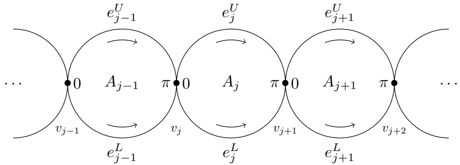

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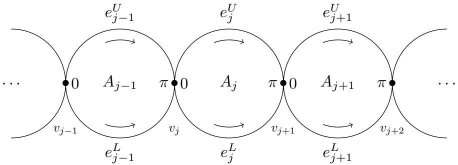

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This is a particular case of the general conditions that make the operator self-adjoint [Kostrykin-Schrader'03]

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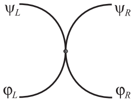
- Without loss of generality we may suppose that the circumference of each ring is 2π, and as usual we employ units in which we have $\hbar = 2m = e = c = 1$, where e is electron charge (forget $\frac{e^2}{\hbar c} = \frac{1}{137}$)

Floquet-Bloch analysis of the fully periodic case



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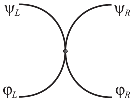

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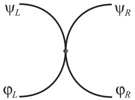

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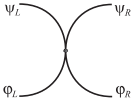

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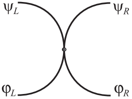

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Apart from the cases $A - \frac{1}{2} \in \mathbb{Z}$ and $k \in \mathbb{N}$ we have $k^2 \in \sigma(-\Delta_\alpha)$ *iff* the condition $|\xi(k)| \leq 1$ is satisfied.

The fully periodic case, continued

Theorem (E-Manko'15)

Let $A \notin \mathbb{Z}$. If $A - \frac{1}{2} \in \mathbb{Z}$, then the spectrum of $-\Delta_\alpha$ consists of two series of infinitely degenerate ev's $\{k^2 \in \mathbb{R} :\, \xi(k) = 0\}$ and $\{k^2 \in \mathbb{R} :\, k \in \mathbb{N}\}$. On the other hand, if $A - \frac{1}{2} \notin \mathbb{Z}$, the spectrum of $-\Delta_\alpha$ consists of infinitely degenerate eigenvalues k^2 with $k \in \mathbb{N}$, and absolutely continuous spectral bands. Each of these bands except the first one is contained in an interval $(n^2, (n+1)^2)$ with $n \in \mathbb{N}$. The first band is included in $(0,1)$ if $\alpha > 4(|\cos A\pi| - 1)/\pi$, or it is negative if $\alpha < -4(|\cos A\pi| + 1)/\pi$, otherwise it contains the point $k^2 = 0$.

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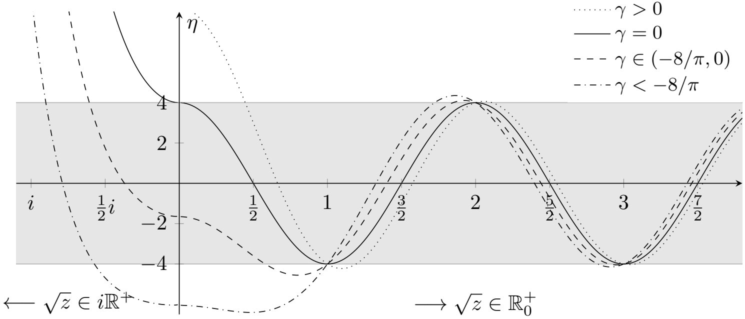
Remarks: (a) We ignore the case $A \in \mathbb{Z}$ which is by a simple gauge transformation equivalent to the non-magnetic case, $A = 0$
(b) In contrast to 'Dirichlet' eigenfunctions with one ring as an 'elementary cell', the 'other' eigenvalues arising for $A - \frac{1}{2} \in \mathbb{Z}$ are supported by *two adjacent rings*

In picture: determining the spectral bands



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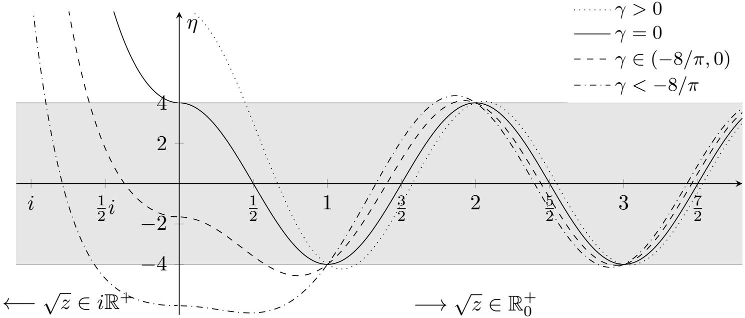

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For $A - \frac{1}{2} \notin \mathbb{Z}$ the situation is similar, just the width of the band changes to $4\cos A\pi$, on the other hand, for $A - \frac{1}{2} \in \mathbb{Z}$ it *shrinks to a line*

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A useful tool to treat them is to rephrase the problem as a system of *difference equation*

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with the components referring to the upper and lower part of Γ, on the other hand the difference one

$$\psi_{j+1}(k) + \psi_{j-1}(k) = \xi_j(k)\psi_j(k)\,, \quad k \in \mathfrak{K}\,,$$

where $\psi_j(k) := \psi(j\pi, k)$ and $\xi(k)$ was introduced above, ξ_j corresponding the coupling α_j. The two equations are intimately related.

Duality, continued

Theorem

Let $\alpha_j \in \mathbb{R}$, *then any solution* $\begin{pmatrix} \psi(\cdot,k) \\ \varphi(\cdot,k) \end{pmatrix}$ *with* $k^2 \in \mathbb{R}$ *and* $k \in \mathfrak{K}$ *satisfies the difference equation, and conversely, the latter defines via*

$$\begin{pmatrix} \psi(x,k) \\ \varphi(x,k) \end{pmatrix} = \mathrm{e}^{\mp iA(x-j\pi)} \Big[\psi_j(k) \cos k(x-j\pi)$$

$$+ (\psi_{j+1}(k)\mathrm{e}^{\pm iA\pi} - \psi_j(k)\cos k\pi) \frac{\sin k(x-j\pi)}{\sin k\pi} \Big], \quad x \in (j\pi,(j+1)\pi)\,,$$

solutions to the former satisfying the δ*-coupling conditions. In addition, the former belongs to* $L^p(\Gamma)$ *if and only if* $\{\psi_j(k)\}_{j\in\mathbb{Z}} \in \ell^p(\mathbb{Z})$*, the claim being true for both* $p \in \{2,\infty\}$.

Local perturbation examples

Consider first non-magnetic perturbations. We skip the theory referring to [Duclos-E-Turek'08, E-Manko'15] and show just examples of the results

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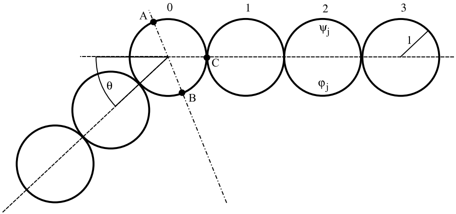

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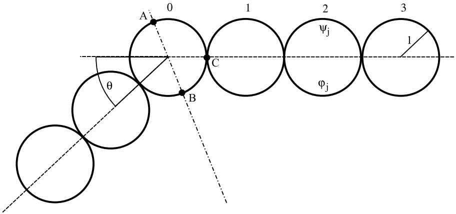
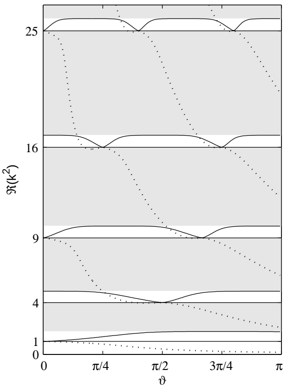


and ask how the spectrum depends on the angle ϑ. In this example we suppose that the magnetic field is absent

In picture: bent-chain spectrum for $\alpha = 3$



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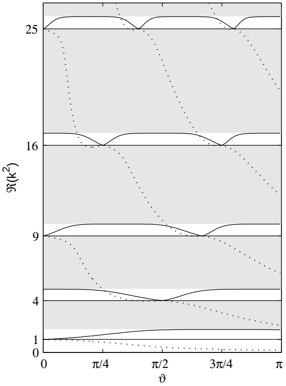

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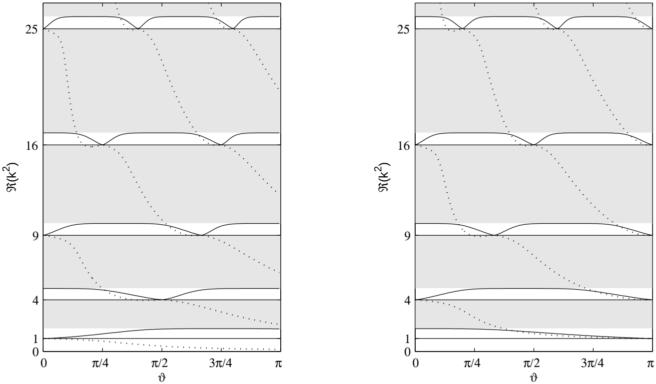

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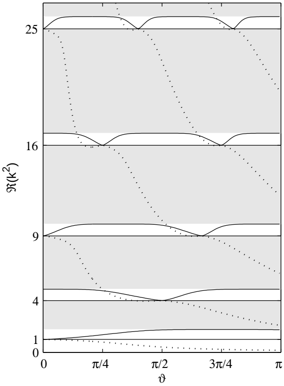

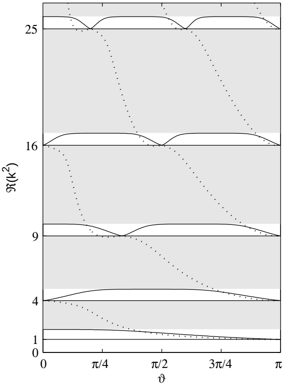

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Similar pictures we get for other values of α, the dotted lines in the figures mark (real values) of resonance positions

We see that the eigenvalues in gaps may be absent but only at rational values of ϑ and never simultaneously

Example: a single coupling constant changed

Let the couplings be $\{\dots, \alpha, \alpha + \gamma_1, \alpha, \dots\}$ and $A \notin \mathbb{Z}$, then we have

Proposition ([E-Manko'15])

Let $A \notin \mathbb{Z}$. The essential spectrum of $-\Delta_{\alpha+\gamma,A}$ coincides with that of $-\Delta_\alpha$. If $\gamma_1 < 0$ there is precisely one simple impurity state in every odd gap, on the other hand, for $\gamma_1 > 0$ there is precisely one simple impurity state in every even gap.

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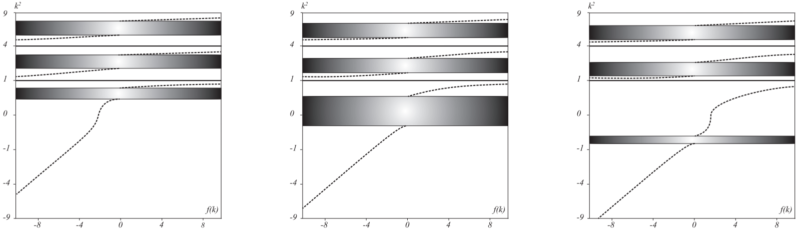

The energy k^2 *vs.* $\gamma_1=f(k)$ for $\cos A\pi=0.6$ and the coupling strength (i) $\alpha=1$, (ii) $\alpha=-1$, (iii) $\alpha=-3$

More general duality

We may consider more general chain graphs, for instance, the magnetic field may vary, $A = \{A_j\}_{j\in\mathbb{Z}}$,

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What is important, the above *duality holds again*, with the difference relation being

$$\begin{aligned}\sin(k\ell_{j-1})\cos(A_j\ell_j)\psi_{j+1}(k) + \sin(k\ell_j)\cos(A_{j-1}\ell_{j-1})\psi_{j-1}(k) \\ = \Big(\frac{\alpha}{2k}\sin(k\ell_{j-1})\sin(k\ell_j) + \sin k(\ell_{j-1}+\ell_j)\Big)\psi_j(k)\,, \quad k \in \mathfrak{K}\,,\end{aligned}$$

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where $\psi_j(k) := \psi(x_j,k)$, and the reconstruction formula becomes

$$\begin{aligned}\begin{pmatrix}\psi(x,k)\\ \varphi(x,k)\end{pmatrix} &= \mathrm{e}^{\mp iA_j(x-x_j)}\Big[\psi_j(k)\cos k(x-x_j) \\ &\quad + (\psi_{j+1}(k)\mathrm{e}^{\pm iA_j\ell_j} - \psi_j(k)\cos k\ell_j)\frac{\sin k(x-x_j)}{\sin k\ell_j}\Big]\,, \quad x\in(x_j,x_{j+1})\,,\end{aligned}$$

Example again: a single flux altered

We suppose that the field is modified on a single ring, i.e. $A = \{\dots, A, A_1, A \dots\}$, the we have a single simple eigenvalue in each gap provided [E-Manko'17]

$$\frac{|\cos A_1\pi|}{|\cos A\pi|} > 1\,,$$

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Can periodic graphs have "wilder" spectra?

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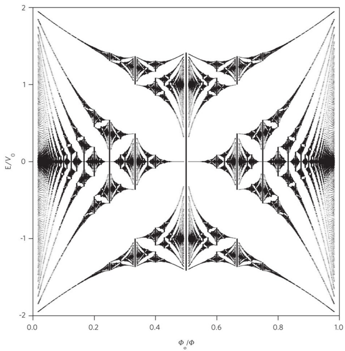

representing the spectrum of the difference operator associated with the *almost Mathieu equation*

$$u_{n+1} + u_{n-1} + 2\lambda \cos(2\pi(\omega + n\alpha))u_n = \epsilon u_n$$

for $\lambda = 1$, otherwise called *Harper equation*, as a function of α

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Fractal nature of spectra for electron on a lattice in a homogeneous magnetic field was conjectured by [Azbel'64] but it caught the imagination only after Hofstadter made the structure visible

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Only recently an experimental realization of the original concept was achieved using a graphene lattice [Dean et al'13], [Ponomarenko'13]

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We exclude the Dirichlet eigenvalues, $\sigma_D = \{k^2 :\ k \in \mathbb{N}\}$, and introduce

$$s(x;z) = \begin{cases} \frac{\sin(x\sqrt{z})}{\sqrt{z}} & \text{for } z \neq 0, \\ x & \text{for } z = 0, \end{cases} \quad \text{and} \quad c(x;z) = \cos(x\sqrt{z})$$

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Theorem (after Pankrashkin'13)

For any interval $J \subset \mathbb{R} \setminus \sigma_D$, the operator $(H_{\gamma,A})_J$ is unitarily equivalent to the pre-image $\eta^{(-1)}\big((L_A)_{\eta(J)}\big)$, where L_A is the operator on $\ell^2(\mathbb{Z})$ acting as $(L_A q\varphi)_j = 2\cos(A_j\pi)\varphi_{j+1} + 2\cos(A_{j-1}\pi)\varphi_{j-1}$ and

$$\eta(z) := \gamma s(\pi;z) + 2c(\pi;z) + 2s'(\pi;z)$$

Non-constant magnetic field, continued

Corollary

The spectrum of $-\Delta_{\gamma,A}$ *is bounded from below and can be decomposed into the discrete set* $\sigma_D = \{n^2 |\, n \in \mathbb{N}\}$ *of infinitely degenerate eigenvalues and the part* σ_{L_A} *determined by* L_A, $\sigma(-\Delta_{\gamma,A}) = \sigma_p \cup \sigma_{L_A}$, *where* σ_{L_A} *can be written as the union*

$$\sigma_{L_A} = \bigcup_{n=0}^{\infty} \sigma_n$$

with $\sigma_n = \eta^{(-1)}\big(\sigma(L_A)\big) \cap I_n$ *for* $n \geq 0$, $I_n = \eta^{(-1)}\big([-4,4]\big) \cap \big(n^2, (n+1)^2\big)$ *for* $n > 0$, *and* $I_0 = \eta^{(-1)}\big([-4,4]\big) \cap \big(-\infty, 1\big)$.

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When $\gamma \neq 0$, *the spectrum has always gaps between the* σ_n*'s. For* $\gamma > 0$, *the spectrum is positive. For* $\gamma < -8\pi$, *the spectrum has a negative part and does not contain zero. Finally,* $0 \in \sigma(-\Delta_{\gamma,A})$ *holds if and only if* $\gamma\pi + 4 \in \sigma(L_A)$.

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Pay attention: In general, the σ_n's may *very different* from absolutely continuous spectral bands!

A linear field growth

Suppose now that $A_j = \alpha j + \theta$ holds for some $\alpha, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$. We denote the corresponding operator L_A by $L_{\alpha,\theta}$, i.e.

$$(L_{\alpha,\theta}\varphi)_j = 2\cos\big(\pi(\alpha j + \theta)\big)\varphi_{j+1} + 2\cos\big(\pi(\alpha j - \alpha + \theta)\big)\varphi_{j-1}$$

for all $j \in \mathbb{Z}$. The rational case, $\alpha = p/q$, is easily dealt with.

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Proposition

Assume that $\alpha = p/q$, where p and q are relatively prime. Then

(a) If $\alpha j + \theta + \frac{1}{2} \notin \mathbb{Z}$ for all $j = 0, \dots, q-1$, then $L_{\alpha,\theta}$ has purely ac spectrum that consists of q closed intervals possibly touching at the endpoints. In particular, $\sigma(L_{\alpha,\theta}) = \big[-4|\cos(\pi\theta)|, 4|\cos(\pi\theta)|\big]$ holds if $q = 1$.

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An irrational slope

On the other hand, if $\alpha \notin \mathbb{Q}$ the spectrum of $L_{\alpha,\theta}$ is closely related to that of the almost Mathieu operator $H_{\alpha,\lambda,\theta}$ in the critical situation, $\lambda = 2$, acting as

$$\left(H_{\alpha,\theta,\lambda}\varphi\right)_j = \varphi_{j+1} + \varphi_{j-1} + \lambda \cos(2\pi\alpha j + \theta)\varphi_j$$

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Combining all these results we can describe the spectrum of our original operator in case the magnetic field varies linearly along the chain

The linear-field spectrum

Theorem (E-Vašata'17)

Let $A_j = \alpha j + \theta$ *for some* $\alpha, \theta \in \mathbb{R}$ *and every* $j \in \mathbb{Z}$*. Then for the spectrum* $\sigma(-\Delta_{\gamma,A})$ *the following holds:*

(a) *If* $\alpha, \theta \in \mathbb{Z}$ *and* $\gamma = 0$*, then* $\sigma(-\Delta_{\gamma,A}) = \sigma_{ac}(-\Delta_{\gamma,A}) \cup \sigma_{pp}(-\Delta_{\gamma,A})$ *where* $\sigma_{ac}(-\Delta_{\gamma,A}) = [0, \infty)$ *and* $\sigma_{pp}(-\Delta_{\gamma,A}) = \{n^2 |\, n \in \mathbb{N}\}$*.*

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(b) *If $\alpha = p/q$ with p and q relatively prime, $\alpha j + \theta + \frac{1}{2} \notin \mathbb{Z}$ for all $j = 0, \dots, q-1$ and assumptions of (a) do not hold, then $-\Delta_{\gamma,A}$ has infinitely degenerate ev's at the points of $\{n^2 |\, n \in \mathbb{N}\}$ and an ac part of the spectrum in each interval $(-\infty, 1)$ and $\big(n^2, (n+1)^2\big)$, $n \in \mathbb{N}$ consisting of q closed intervals possibly touching at the endpoints.*

The linear-field spectrum

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(c) *If $\alpha = p/q$, where p and q are relatively prime, and $\alpha j + \theta + \frac{1}{2} \in \mathbb{Z}$ for some $j = 0, \dots, q-1$, then the spectrum $-\Delta_{\gamma,A}$ is of pure point type and such that in each interval $(-\infty, 1)$ and $\big(n^2, (n+1)^2\big)$, $n \in \mathbb{N}$ there are exactly q distinct eigenvalues and the remaining eigenvalues form the set $\{n^2 |\, n \in \mathbb{N}\}$. All the eigenvalues are infinitely degenerate.*

The linear-field spectrum, continued

Theorem (E-Vašata'17, cont'd)

(d) *If $\alpha \notin \mathbb{Q}$, then $\sigma(-\Delta_{\gamma,A})$ does not depend on θ and it is a disjoint union of the isolated-point family $\{n^2 |\, n \in \mathbb{N}\}$ and Cantor sets, one inside each interval $(-\infty, 1)$ and $\big(n^2, (n+1)^2\big)$, $n \in \mathbb{N}$. Moreover, the overall Lebesgue measure of $\sigma(-\Delta_{\gamma,A})$ is zero.*

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Using a fresh result of [Last-Shamis'16] we can also show

Proposition

Let $A_j = \alpha j + \theta$ *for some* $\alpha, \theta \in \mathbb{R}$ *and every* $j \in \mathbb{Z}$. *There exist a dense* G_δ *set of the slopes* α *for which, and all* θ, *the Haussdorff dimension*

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Remark: If you regard a linear field *unphysical*, you may either view it as an *idealization* or to replace it a *quasiperiodic function* with the *same slope* leading to *the same result*.

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Berkolaiko and Kuchment say that the situation with graphs is similar, however, they add immediately that *this is not a strict law* and illustrate this claim on resonant gaps created by a graph 'decoration', see also [Schenker-Aizenman'00]

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The answer depends on the vertex coupling. Recall that the standard coupling conditions

$$(U-I)\Psi + i(U+I)\Psi' = 0\,,$$

where Ψ, Ψ' are vectors of values and derivatives at the vertex, U is an $n \times n$ unitary matrix, where n is the vertex degree, decomposes into Dirichlet, Neumann, and Robin parts corresponding to eigenspaces of U with eigenvalues -1, 1, and the rest, respectively; if the latter is absent we call such a coupling *scale-invariant*

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Theorem ([E-Turek'17])

An infinite periodic quantum graph does not belong to the Bethe-Sommerfeld class if the couplings at its vertices are scale-invariant.

Proof idea

The spectrum is determined by *secular equation* [B-K'13]: we define

$$F(k;\vec{\vartheta}) := \det\left(\mathbf{I} - \mathrm{e}^{i(\mathbf{A}+k\mathbf{L})}\mathbf{S}(k)\right),$$

where the $2E \times 2E$ matrices **A**, **L**, and **S** are as follows: the diagonal matrix **L** is given by the lengths of the directed edges (bonds) of Γ,

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Recall next that the vertex conditions can be equivalently written as

$$\begin{pmatrix} I^{(r)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-r)} \end{pmatrix} \Psi$$

for certain r, S, and T, where $I^{(r)}$ is the identity matrix of order r; the coupling is scale-invariant if and only if the square matrix $S = 0$

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We will consider two *associated* quantum graph Hamiltonians, H with the above vertex coupling, and H_0 where we replace S by zero

A result for this associated pair

Proposition ([E-Turek'17])

For the spectra $\sigma(H)$ and $\sigma(H_0)$ the following claims hold true:

(i) *If $\sigma(H_0)$ has an open gap, then $\sigma(H)$ has infinitely many gaps.*

(ii) *If the edge lengths are rationally dependent, then the gaps of $\sigma(H)$ asymptotically coincide with those of $\sigma(H_0)$.*

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The same is true for $\mathbf{S}(k)$, and as consequence, the spectrum at high energies is mostly determined by the scale-invariant part. □

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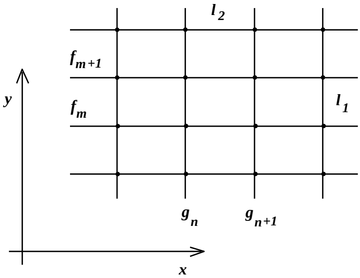
As usual with existence claims, it is enough to demonstrate an example. With this aim we are going to revisit the model of a *rectangular lattice graph* introduced in [E'96, E-Gawlista'96]



Spectral condition

According to [E'96], a number $k^2 > 0$ belongs to a gap if and only if $k > 0$ satisfies the gap condition, which reads

$$\tan\left(\frac{ka}{2} - \frac{\pi}{2}\left\lfloor\frac{ka}{\pi}\right\rfloor\right) + \tan\left(\frac{kb}{2} - \frac{\pi}{2}\left\lfloor\frac{kb}{\pi}\right\rfloor\right) < \frac{\alpha}{2k} \quad \text{for } \alpha > 0$$

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where we denote the edge lengths ℓ_j, $j = 1, 2$, as a, b; we neglect the Kirchhoff case, $\alpha = 0$, where $\sigma(H) = [0, \infty)$.

Note that for $\alpha < 0$ the spectrum extends to the negative part of the real axis and may have a gap there, which is not important here because there is not more than a single negative gap, and this gap *always extends to positive values*

What is known

The spectrum depends on the ratio $\theta = \frac{\ell_1}{\ell_2}$. If θ is rational, $\sigma(H)$ has infinitely many gaps unless $\alpha = 0$ in which case $\sigma(H) = [0, \infty)$

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On the other hand, $\theta \in \mathbb{R}$ is *badly approximable* if there is a $c > 0$ such that

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for all $p, q \in \mathbb{Z}$ with $q \neq 0$. For such numbers we define the *Markov constant* by

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(we note that $\mu(\theta) = \mu(\theta^{-1})$) and its *'one-sided analogues'*

The golden mean situation

Let us start with the *golden mean*, $\phi = \frac{\sqrt{5}+1}{2} = [1; 1, 1, \dots]$, which can be regarded as the 'worst' irrational

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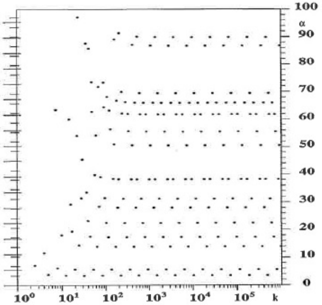

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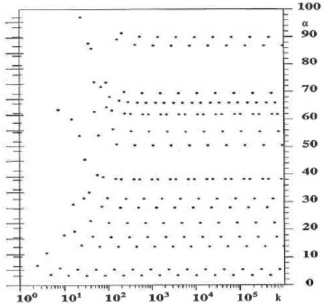

Note that they approach the limit values *from above*, also that the series open at $\frac{\pi^2}{\sqrt{5ab}}\phi^{\pm 1/2}|n^2 - m^2 - nm|,\; n,m \in \mathbb{N}$ [E-Gawlista'96]

But a closer look shows a more complex picture

Theorem ([E-Turek'17])

Let $\frac{a}{b} = \phi = \frac{\sqrt{5}+1}{2}$, then the following claims are valid:

(i) *If $\alpha > \frac{\pi^2}{\sqrt{5}a}$ or $\alpha \le -\frac{\pi^2}{\sqrt{5}a}$, there are infinitely many spectral gaps.*

(ii) *If*

$$-\frac{2\pi}{a}\tan\left(\frac{3-\sqrt{5}}{4}\pi\right) \le \alpha \le \frac{\pi^2}{\sqrt{5}a},$$

there are no gaps in the positive spectrum.

(iii) *If*

$$-\frac{\pi^2}{\sqrt{5}a} < \alpha < -\frac{2\pi}{a}\tan\left(\frac{3-\sqrt{5}}{4}\pi\right),$$

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Corollary

The above theorem about the existence of BS graphs is valid.

More about this example

The window in which the golden-mean lattice has the Bethe–Sommerfeld property is narrow, it is roughly $4.298 \lesssim -\alpha a \lesssim 4.414$.

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We are also able to control the number of gaps in the BS regime:

Theorem ([E-Turek'17])

For a given $N \in \mathbb{N}$, there are exactly N gaps in the positive spectrum if and only if α is chosen within the bounds

$$-\frac{2\pi\left(\phi^{2(N+1)}-\phi^{-2(N+1)}\right)}{\sqrt{5}a}\tan\left(\frac{\pi}{2}\phi^{-2(N+1)}\right) \le \alpha < -\frac{2\pi\left(\phi^{2N}-\phi^{-2N}\right)}{\sqrt{5}a}\tan\left(\frac{\pi}{2}\phi^{-2N}\right).$$

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Note that the numbers $A_j := \frac{2\pi\left(\phi^{2j}-\phi^{-2j}\right)}{\sqrt{5}}\tan\left(\frac{\pi}{2}\phi^{-2j}\right)$ form an increasing sequence the first element of which is $A_1 = 2\pi\tan\left(\frac{3-\sqrt{5}}{4}\pi\right)$ and

$$A_j < \frac{\pi^2}{\sqrt{5}} \quad \text{for all } j \in \mathbb{N}.$$

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Proofs of the above results are based on properties of Diophantine approximations. In a similar way one can prove

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Let $\theta = \frac{a}{b}$ and define

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and γ_- similarly with $\lfloor\cdot\rfloor$ replaced by $\lceil\cdot\rceil$. If the coupling constant α satisfies

$$\gamma_\pm < \pm\alpha < \frac{\pi^2}{\max\{a, b\}}\mu(\theta)\,,$$

then there is a nonzero and finite number of gaps in the positive spectrum.

BS property does not need a definite sign of α

Proposition ([E-Turek'17])

Let the edge ratio be

$$\theta = \frac{2t^3 - 2t^2 - 1 + \sqrt{5}}{2(t^4 - t^3 + t^2 - t + 1)} \quad \text{for} \quad t \in \mathbb{N},\ t \geq 3\,;$$

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Note that the above number θ can be written as $\theta = \frac{t\phi+1}{(t^2+1)\phi+t}$ with $\phi = \frac{1+\sqrt{5}}{2}$, and moreover, the continued-fraction representation of θ is $[0; t, t, 1, 1, 1, 1, \dots]$. Furthermore, we have $\mu(\theta) = \mu(\phi) = \frac{1}{\sqrt{5}}$.

The talk was based on

[EM15] P.E., Stepan Manko: Spectra of magnetic chain graphs: coupling constant perturbations, *J. Phys. A: Math. Theor.* **48** (2015), 125302 (20pp)

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as well as the other papers mentioned in the course of the presentation.

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Thank you for your attention!