Stability of closed gaps for the alternating Kronig-Penney Hamiltonian

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Outline of the presentation

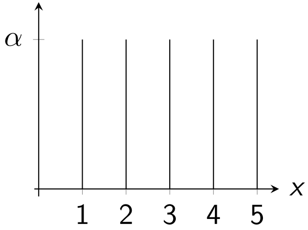
1. Alternating Kronig-Penney Hamiltonian
   - Generalized KP
   - Spectral properties of gKP
   - Spectral gaps of the aKP
2. Approximation with finite range interactions
3. Norm resolvent convergence of H_ε to $-\Delta_\alpha$
4. Future directions

Kronig-Penney (KP) Hamiltonian

1d crystal with point interactions $\Longrightarrow$ Kronig-Penney model

$$H_{\mathrm{KP}} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \alpha \sum_{n \in \mathbb{Z}} \delta(x - n)$$

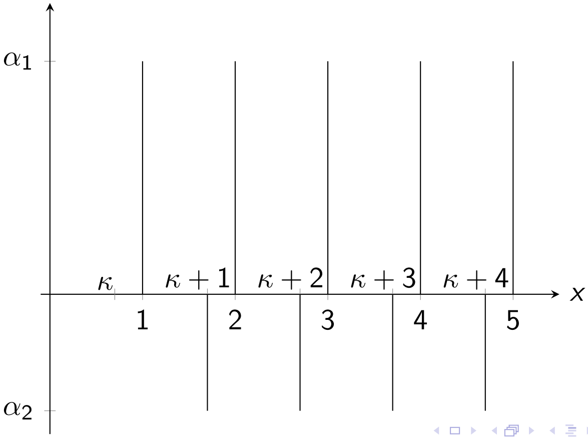
- idealization of very-short-range, strong interactions
- reasonably accurate approximation of finite-range periodic models
- depends only on the interaction strength α
- exact analytic solution and fast numerics



Generalized KP (gKP) Hamiltonian

Generalized (two-species) Kronig-Penney model

$$H_{\alpha_1,\alpha_2,\kappa} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \alpha_1 \sum_{n\in\mathbb{Z}} \delta(x-n) + \alpha_2 \sum_{n\in\mathbb{Z}} \delta(x-\kappa-n), \qquad \kappa \in (0,1)$$



Can be described in terms of boundary conditions on the lattice

$$\mathcal{Z}_\kappa = \mathbb{Z} \cup (\mathbb{Z} + \kappa), \quad \kappa \in (0,1)$$

$$-\Delta_{\alpha_1,\alpha_2,\kappa} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

$$\mathcal{D}(-\Delta_{\alpha_1,\alpha_2,\kappa}) = \left\{ \begin{array}{c} \psi \in H^2(\mathbb{R} \setminus \mathcal{Z}_\kappa) \cap H^1(\mathbb{R}) \\ \text{such that } \forall n \in \mathbb{Z} \\ \psi'(n^+) - \psi'(n^-) = \alpha_1 \psi(n) \\ \psi'((n+\kappa)^+) - \psi'((n+\kappa)^-) = \alpha_2 \psi(n+\kappa) \end{array} \right\}$$

Associated quadratic form

$$Q_{\alpha_1,\alpha_2,\kappa}[\varphi,\psi] = \int_{\mathbb{R}} \overline{\varphi}' \, \psi' \, \mathrm{d}x + \alpha_1 \sum_{n\in\mathbb{Z}} \overline{\varphi(n)} \, \psi(n) + \alpha_2 \sum_{n\in\mathbb{Z}} \overline{\varphi(n+\kappa)} \, \psi(n+\kappa)$$

$$\mathcal{D}(Q_{\alpha_1,\alpha_2,\kappa}) = H^1(\mathbb{R})$$

Bloch-Floquet transform

To (partially) diagonalize periodic Hamiltonians, use Bloch-Floquet transform

$$L^2(\mathbb{R}) \xrightarrow{\cong} L^2(\mathbb{Z} \times I) \xrightarrow{\cong} \ell^2(\mathbb{Z}) \otimes L^2(I) \xrightarrow{\mathcal{F} \otimes \mathbf{1}_{L^2(I)}} L^2(\mathbb{T}) \otimes L^2(I)$$

$$U : L^2(\mathbb{R}) \to L^2(\mathbb{T}) \otimes L^2(I)$$

$$\boxed{u_k(x) = (U\psi)_k(x) := \frac{1}{\sqrt{2\pi}} \sum_{n \in \mathbb{Z}} \mathrm{e}^{\mathrm{i}kn} \psi(x-n)} = \mathrm{e}^{-\mathrm{i}k} u_k(x-1)$$

$I = [0,1] =$ unit cell

$k =$ crystal/Bloch momentum

$\mathbb{T} = (-\pi, \pi] =$ Brillouin zone

Fiber Hamiltonian

Identifying

$$L^2(\mathbb{T})\otimes L^2(I) \cong \int_{(-\pi,\pi]}^{\oplus} \mathcal{H}_k \, \frac{\mathrm{d}k}{2\pi}, \quad \mathcal{H}_k := \left\{ u \in L^2_{\mathrm{loc}}(\mathbb{R}) \mid u(x+1) = e^{\mathrm{i}k} u(x) \right\}$$

we have

$$U(-\Delta_{\alpha_1,\alpha_2,\kappa})U^{-1} = \int_{(-\pi,\pi]}^{\oplus} (-\Delta^{(k)}_{\alpha_1,\alpha_2,\kappa}) \, \frac{\mathrm{d}k}{2\pi}$$

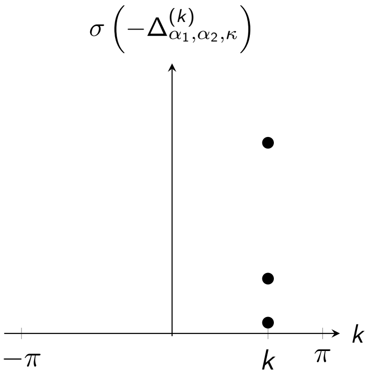
where the fiber Hamiltonian $-\Delta^{(k)}_{\alpha_1,\alpha_2,\kappa}$ is

$$-\Delta^{(k)}_{\alpha_1,\alpha_2,\kappa} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

$$\mathcal{D}(-\Delta^{(k)}_{\alpha_1,\alpha_2,\kappa}) = \left\{ \begin{array}{c} u \in \mathcal{H}_k \text{ s.t. } u\big|_{(0,1)} \in H^2((0,1) \setminus \{\kappa\}), \\ u \in C(\mathbb{R}), \text{ and } \forall n \in \mathbb{Z} \\ u'(n^+) - u'(n^-) = \alpha_1 \, u(n) \\ u'((n+\kappa)^+) - u'((n+\kappa)^-) = \alpha_2 \, u(n+\kappa) \end{array} \right\}$$

Spectral properties of $-\Delta^{(k)}_{\alpha_1,\alpha_2,\kappa}$

Spectral properties of $-\Delta^{(k)}_{\alpha_1,\alpha_2,\kappa}$ determine the ones of $-\Delta_{\alpha_1,\alpha_2,\kappa}$



Theorem ([Yoshitomi (2006)])

$-\Delta^{(k)}_{\alpha_1,\alpha_2,\kappa}$ *has purely discrete spectrum for each* $k \in (-\pi, \pi]$

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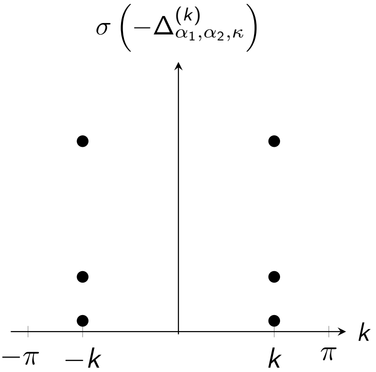

Theorem ([Yoshitomi (2006)])

$-\Delta^{(k)}_{\alpha_1,\alpha_2,\kappa}$ and $-\Delta^{(-k)}_{\alpha_1,\alpha_2,\kappa}$ are antiunitarily equivalent under ordinary complex conjugation, whence in particular their eigenvalues are identical and their eigenfunctions are complex conjugate

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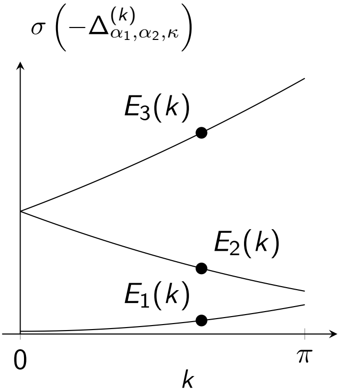

Theorem ([Yoshitomi (2006)])

Denoting by $E_\ell(k)$, $\ell = 1, 2, \dots,$ the ℓ-th eigenvalue of $-\Delta^{(k)}_{\alpha_1,\alpha_2,\kappa}$ when $k \in [0, \pi]$ (labelled in increasing order), each map $[0, \pi] \ni k \mapsto E_\ell(k)$ is analytic on $(0, \pi)$, continuous at $k = 0$ and $k = \pi$, monotone increasing for ℓ odd, and monotone decreasing for ℓ even

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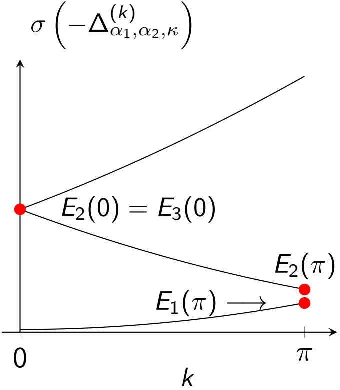

Theorem ([Yoshitomi (2006)])

All $E_\ell(k)$'s are non-degenerate whenever $k \in (0,\pi)$ and, because of (iii), at most twice degenerate when $k = 0$ or $k = \pi$

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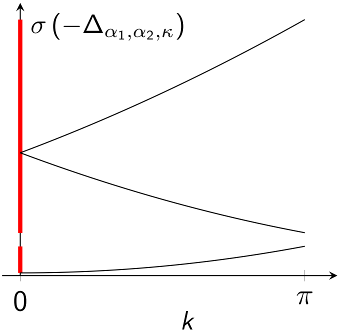


Theorem ([Yoshitomi (2006)])

The spectrum $\sigma(-\Delta_{\alpha_1,\alpha_2,\kappa})$ of $-\Delta_{\alpha_1,\alpha_2,\kappa}$ is purely absolutely continuous and has the structure

$$\sigma(-\Delta_{\alpha_1,\alpha_2,\kappa}) = \bigcup_{\ell=1}^{\infty} E_\ell([0,\pi])$$

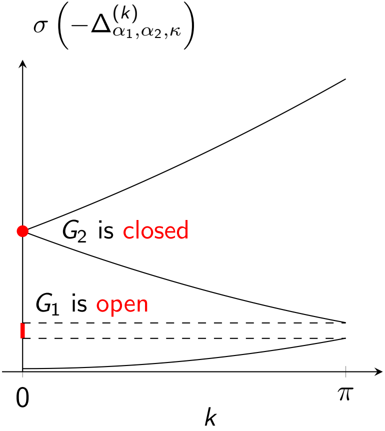
Spectral gaps

$$G_\ell := \begin{cases} (E_\ell(\pi), E_{\ell+1}(\pi)) & \ell \text{ odd} \\ (E_\ell(0), E_{\ell+1}(0)) & \ell \text{ even} \end{cases}$$

ℓ-th spectral gap of $-\Delta_{\alpha_1,\alpha_2,\kappa}$

closed gap $\to$ conduction

open gap $\to$ insulation



Characterization of gaps of $-\Delta_{\alpha_1,\alpha_2,\kappa}$

Theorem ([Yoshitomi (2006)])

Let $-\Delta_{\alpha_1,\alpha_2,\kappa}$ be the gKP Hamiltonian and let G_ℓ, $\ell = 1, 2, \ldots,$ be the gaps in its spectrum.

(i) *If $\alpha_2 \neq -\alpha_1$ or $\kappa \notin \mathbb{Q}$, then all gaps are open.*

(ii) *If $\alpha_2 = -\alpha_1$ and $2\kappa = m/n$ for two relatively prime integers $m, n \in \mathbb{N}$ such that m is not even, then*

$$G_\ell = \emptyset \quad \text{for } \ell \in 2n\mathbb{N}, \qquad G_\ell \neq \emptyset \quad \text{for } \ell \notin 2n\mathbb{N}.$$

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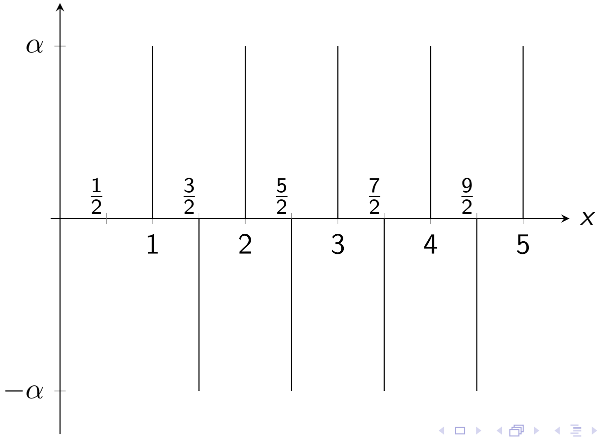
Alternating KP (aKP) Hamiltonian

We focus on the alternating Kronig-Penney model

$$-\Delta_\alpha = -\Delta_{\alpha,-\alpha,1/2} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \alpha \sum_{n\in\mathbb{Z}} \left[\delta(x-n) - \delta(x-1/2-n)\right], \quad \alpha > 0$$



Gaps of aKP

The above Theorem of Yoshitomi gives

Corollary

The even gaps of $-\Delta_\alpha$ are all closed. *The odd gaps of $-\Delta_\alpha$ are all open.*

Proof: analysis of discriminant of corresponding ODE and its monodromy matrix (tedious)

Problem

Is the vanishing of all the gaps at the centre of the Brillouin zone in the spectrum of $-\Delta_\alpha$ an exceptional occurrence of the idealised model of delta-interactions, or is it instead a structural property that is also present in some approximating "physical" model of alternating periodic interactions of finite (non-zero) range?

Example: Thomas effect

Gaps of aKP

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Example: Thomas effect

AGHK potential

Standard approximation: [Albeverio–Gesztesy–Høegh-Krohn–Kirsch (1984)]

$$V_\varepsilon^{\mathrm{AGHK}}(x) := \sum_{n\in\mathbb{Z}} (-1)^n \frac{\alpha}{\varepsilon} V\left(\frac{x-n/2}{\varepsilon}\right), \quad \varepsilon > 0$$

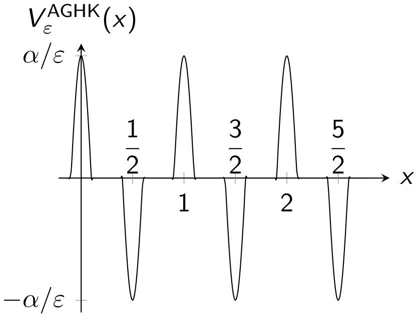
$V \in L^1(\mathbb{R})$, $\int_{\mathbb{R}} V(x)\,\mathrm{d}x = 1$

Theorem ([AGHK (1988)])

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_\varepsilon^{AGHK} \xrightarrow[\varepsilon\to 0]{\|\cdot\|_{\mathrm{res}}} -\Delta_\alpha$$

Corollary

$$\sigma\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_\varepsilon^{AGHK}\right) \xrightarrow[\varepsilon\to 0]{} \sigma(-\Delta_\alpha)$$



Main result

Caveat

The even gaps of $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_\varepsilon^{\mathrm{AGHK}}$ are not all closed!

Theorem ([Michelangeli–M., *Anal. Math. Phys.* (2015)])

It is always possible to modify each bump of V_ε^{AGHK} by adding to it a small correction, with the same support but with peak magnitude of order 1 in ε, in such a way that the resulting modified bump-like potential $\widetilde{V}_\varepsilon^{AGHK}$ has the following properties: for each ε, all the gaps at the centre of the Brillouin zone for the spectrum of $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \widetilde{V}_\varepsilon^{AGHK}$ vanish, and as $\varepsilon \to 0$ the operator $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \widetilde{V}_\varepsilon^{AGHK}$ too converges to $-\Delta_\alpha$ in the norm resolvent sense.

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Auxiliary result

Theorem ([Michelangeli–Zagordi (2009)])

Let V be a continuous, real-valued potential with period 1. Then $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$ has all even gaps closed if and only if

$$V(x) = v_0 + W^2(x) + W'(x)$$

for some constant $v_0 \in \mathbb{R}$ and some C^1-function W such that

$$W\left(x + \frac{1}{2}\right) = -W(x) \qquad \forall x \in \mathbb{R}.$$

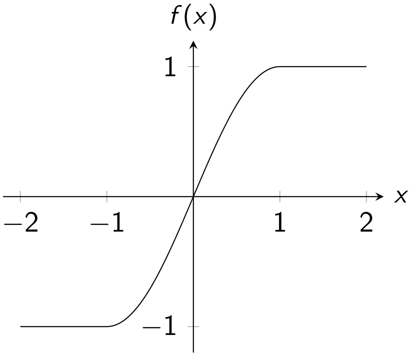
If this is the case, then $v_0 = \int_0^1 \left[V(x) - W^2(x)\right] \mathrm{d}x$ and

$$W(x) = -\frac{1}{2} \int_x^{x+\frac{1}{2}} \left[V(y) - \int_0^1 V(t)\,\mathrm{d}t\right] \mathrm{d}y.$$

Approximating potential V_ε

Strategy: construct approximating potential $V_\varepsilon = \widetilde{V}_\varepsilon^{\mathrm{AGHK}}$ in the form above

Pick $f \in C^1(\mathbb{R})$ s.t. $f(x) \equiv -1$ for $x \leq -1$ and $f(x) \equiv 1$ for $x \geq 1$

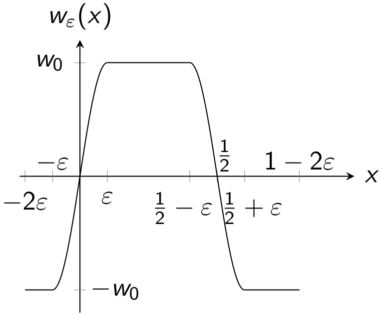


Approximating potential V_ε

Strategy: construct approximating potential $V_\varepsilon = \widetilde{V}_\varepsilon^{\mathrm{AGHK}}$ in the form above

For a fixed $w_0 \in \mathbb{R}$ define

$$w_\varepsilon(x) := \begin{cases} w_0\, f\left(\dfrac{x}{\varepsilon}\right) & -2\varepsilon \le x \le 2\varepsilon, \\ w_0 & 2\varepsilon \le x \le \dfrac{1}{2} - 2\varepsilon, \\ -w_\varepsilon\left(x - \frac{1}{2}\right) & \dfrac{1}{2} - 2\varepsilon \le x \le 1 - 2\varepsilon \end{cases}$$



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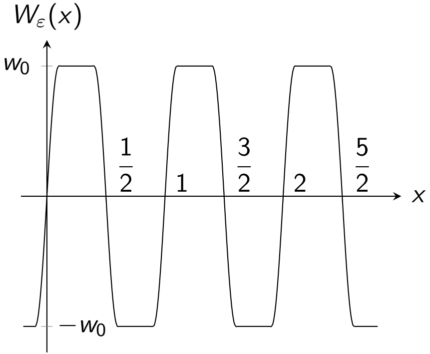
Strategy: construct approximating potential $V_\varepsilon = \widetilde{V}_\varepsilon^{\mathrm{AGHK}}$ in the form above

Extend it by periodicity:

$$W_\varepsilon(x) := w_\varepsilon(y)$$

if $x = y + n$ for some $y \in [-2\varepsilon, 1 - 2\varepsilon]$ and $n \in \mathbb{Z}$



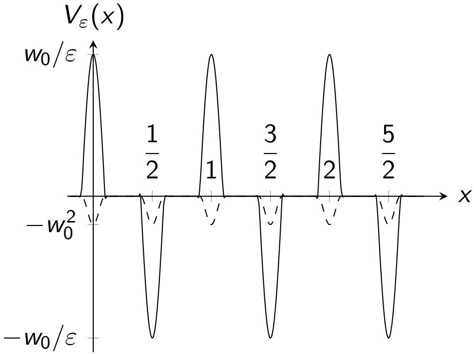
Approximating potential V_ε

Strategy: construct approximating potential $V_\varepsilon = \widetilde{V}_\varepsilon^{\mathrm{AGHK}}$ in the form above

Set

$$V_\varepsilon(x) := -w_0^2 + W_\varepsilon(x)^2 + W'_\varepsilon(x)$$
$$= V_\varepsilon^{(1)}(x) + \varepsilon\, V_\varepsilon^{(2)}(x)$$

———	$V_\varepsilon^{(1)}(x)$
- - - - -	$\varepsilon\, V_\varepsilon^{(2)}(x)$



Structure of V_ε

$$V_\varepsilon^{(1)}(x) = \sum_{n\in\mathbb{Z}} U_{\varepsilon,n}^{(1)}\left(x - \frac{n}{2}\right)$$

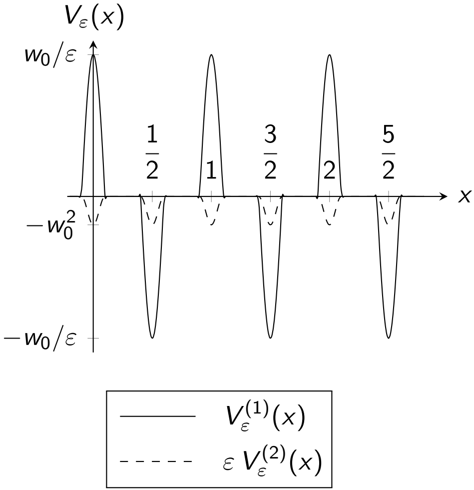
$$U_{\varepsilon,n}^{(1)}(x) := \frac{1}{\varepsilon} U_n^{(1)}\left(\frac{x}{\varepsilon}\right),$$

$$U_n^{(1)}(x) := (-1)^n\, w_0\, f'(x),$$

$$V_\varepsilon^{(2)}(x) = \sum_{n\in\mathbb{Z}} U_\varepsilon^{(2)}\left(x - \frac{n}{2}\right),$$

$$U_\varepsilon^{(2)}(x) := \frac{1}{\varepsilon} U^{(2)}\left(\frac{x}{\varepsilon}\right),$$

$$U^{(2)}(x) := w_0^2\left(f^2(x) - 1\right)$$



Spectral gaps of $V_\varepsilon^{\mathrm{AGHK}}$

The result by Michelangeli–Zagordi gives that $H_\varepsilon = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_\varepsilon$ has all even gaps closed

On the contrary, the even gaps of $-\dfrac{\mathrm{d}^2}{\mathrm{d}x^2} + V_\varepsilon^{\mathrm{AGHK}}$ are not all closed!

If that was the case

$$V_\varepsilon^{\mathrm{AGHK}}(x) = v_{\varepsilon,0}^{\mathrm{AGHK}} + W_\varepsilon^{\mathrm{AGHK}}(x)^2 + \frac{\mathrm{d}}{\mathrm{d}x} W_\varepsilon^{\mathrm{AGHK}}(x)$$

with

$$\frac{\mathrm{d}}{\mathrm{d}x} W_\varepsilon^{\mathrm{AGHK}}(x) = \frac{1}{2}\left(V_\varepsilon^{\mathrm{AGHK}}(x) - V_\varepsilon^{\mathrm{AGHK}}(x+1/2)\right) = V_\varepsilon^{\mathrm{AGHK}}(x)$$

$$\implies W_\varepsilon^{\mathrm{AGHK}}(x) \equiv \mathrm{const} \quad \implies \quad V_\varepsilon^{\mathrm{AGHK}}(x) \equiv 0 \perp$$

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Convergence $H_\varepsilon \to -\Delta_\alpha$

Theorem (Main result, rephrased)

Let $w_0 = \alpha/2$. *Then*

$$H_\varepsilon = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_\varepsilon \xrightarrow[\varepsilon\to 0]{\|\cdot\|_{\mathrm{res}}} -\Delta_\alpha$$

Proof

- $H_\varepsilon = H_\varepsilon^{\mathrm{AGHK}} + \varepsilon V_\varepsilon^{(2)}$
- $H_\varepsilon^{\mathrm{AGHK}} \xrightarrow[\varepsilon\to 0]{\|\cdot\|_{\mathrm{res}}} -\Delta_\alpha$ [AGHK (1988)]
- $\left| V_\varepsilon^{(2)}[\varphi, \psi] \right| \leq c \, \|\varphi\|_{H^1} \, \|\psi\|_{H^1}$ (simple computation)
- $\varepsilon V_\varepsilon^{(2)} \xrightarrow[\varepsilon\to 0]{\|\cdot\|_{\mathrm{res}}} 0$ by [Reed–Simon I (1972)] □

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Future directions

- Generalize the argument of Michelangeli–Zagordi to odd gaps (at $k = \pi$ in the Brillouin zone)
- Obtain smooth, finite range approximants for all gKP Hamiltonians $-\Delta_{\alpha_1,\alpha_2,\kappa}$; recover Yoshitomi's results
- Physical consequences: conduction in two-species $1d$ crystals