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Stability of closed gaps for the alternating Kronig–Penney Hamiltonian

Alessandro Michelangeli^{1,2} · Domenico Monaco²

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Abstract We consider the Kronig–Penney model for a quantum crystal with equispaced periodic delta-interactions of alternating strength. For this model all spectral gaps at the centre of the Brillouin zone are known to vanish, although so far this noticeable property has only been proved through a very delicate analysis of the discriminant of the corresponding ODE and the associated monodromy matrix. We provide a new, alternative proof by showing that this model can be approximated, in the norm resolvent sense, by a model of regular periodic interactions with finite range for which all gaps at the centre of the Brillouin zone are still vanishing. In particular this shows that the vanishing gap property is stable in the sense that it is present also for the “physical” approximants and is not only a feature of the idealised model of zero-range interactions.

Keywords Kronig–Penney model · Point interactions · Spectral bands and gaps · Convergence of self-adjoint operators

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Domenico Monaco
dmonaco@sissa.it

Alessandro Michelangeli
michel@math.lmu.de; alemiche@sissa.it

¹ Institute of Mathematics, Ludwig Maximilian University of Munich, Theresienstr. 39, 80333 Munich, Germany

² SISSA-International School for Advanced Studies, Via Bonomea 265, 34136 Trieste, Italy

1 Introduction and main results: the problem of the spectral gaps of the alternating Kronig–Penning pseudo-potential

The so-called one-dimensional generalised (two-species) Kronig–Penney (KP) model is an idealised model for a one-dimensional periodic crystal with point (delta-like) interactions, described by the formal Hamiltonian

$$H_{\alpha_1, \alpha_2, \kappa} = -\frac{d^2}{dx^2} + \alpha_1 \sum_{n \in \mathbb{Z}} \delta(x - n) + \alpha_2 \sum_{n \in \mathbb{Z}} \delta(x - \kappa - n), \quad (1.1)$$

where for concreteness a unit period is chosen. The parameters $\alpha_1, \alpha_2 \in \mathbb{R}$ denote the strengths of the delta-interactions supported, respectively, at $x = 0, \pm 1, \pm 2, \dots$ and at $x = \kappa, \kappa \pm 1, \kappa \pm 2, \dots$. The shift κ is assumed to range in $(0, 1)$. The presence of the shifted terms justifies the terminology of generalised KP model, with respect to the original model proposed by Kronig and Penney [12] and extensively studied thereafter (see, e.g., [1, 3, 10, 13]).

Albeit an idealisation of actual periodic interactions with very short range and strong magnitude, Kronig–Penney-like models have always been of high relevance in the theory and the experiments of condensed matter physics [4, 9, 11]: they provide a reasonably accurate approximation of periodic models with finite range with the advantage of depending only on one effective parameter, the interaction strength α , instead of requiring the knowledge of all the interaction details; as such, they allow for an exact analytic solution and fast numerics and they are suited to model a large class of theoretical and experimental setups for polyatomic crystals (see, e.g., [6]).

It is well-known that the delta-interactions in the formal Hamiltonian (1.1) describe in fact suitable boundary conditions at the points of the lattice

$$\mathcal{Z}_\kappa = \{n \mid n \in \mathbb{Z}\} \cup \{n + \kappa \mid n \in \mathbb{Z}\}, \quad \kappa \in (0, 1). \quad (1.2)$$

In turn (1.1) can be given a rigorous realisation as a self-adjoint operator on the natural Hilbert space of the problem, namely $L^2(\mathbb{R})$, and that is the operator we shall refer to hereafter. Explicitly (see, e.g., [1] Chapter III.2 and reference therein), for fixed $\alpha_1, \alpha_2 \in (-\infty, +\infty]$ and $\kappa \in (0, 1)$, the operator $-\Delta_{\alpha_1, \alpha_2, \kappa}$ whose action and domain are defined by¹

$$-\Delta_{\alpha_1, \alpha_2, \kappa} = -\frac{d^2}{dx^2} \quad (1.3)$$

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

¹ We shall adopt the following notation. By $H^k(J)$ we shall denote the k -th Sobolev space on the interval J . The domain of an operator T will be denoted by $\mathcal{D}(T)$ and in case T is a self-adjoint operator we shall denote its quadratic form and its form domain, respectively, by $T[\cdot, \cdot]$ and $\mathcal{D}[T]$ (see, e.g., [21]). $L^2_{\text{loc}}(\mathbb{R})$ will denote the space of functions on \mathbb{R} that on each compact are square-integrable. Non-negative multiplicative constants (that do not depend on the other quantities under consideration) are denoted by c .

is self-adjoint on $L^2(\mathbb{R})$ with associated quadratic (energy) form given by

$$\begin{aligned} Q_{\alpha_1, \alpha_2, \kappa}[\varphi, \psi] &= \int_{\mathbb{R}} \overline{\varphi'} \psi' \, dx + \alpha_1 \sum_{n \in \mathbb{Z}} \overline{\varphi(n)} \psi(n) \\ &\quad + \alpha_2 \sum_{n \in \mathbb{Z}} \overline{\varphi(n + \kappa)} \psi(n + \kappa) \end{aligned} \tag{1.4}$$

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

The operator $-\Delta_{\alpha_1, \alpha_2, \kappa}$ is customarily referred to as the generalised Kronig–Penney Hamiltonian of point interactions at the sites of the lattice \mathcal{Z}_κ ; from (1.4) one sees that its quadratic form $Q_{\alpha_1, \alpha_2, \kappa}[\varphi, \psi]$ reproduces indeed the formal expectation $\langle \varphi, H_{\alpha_1, \alpha_2, \kappa} \psi \rangle$ obtained from (1.1). A comprehensive overview of the properties of models of infinitely many delta-interactions in one dimension (such as $-\Delta_{\alpha_1, \alpha_2, \kappa}$) and of the related literature may be found in Chapter III.2 of [1].

In this work we are concerned with the spectral properties of certain generalised KP models, namely those that exhibit a peculiar feature of *vanishing spectral gaps*. We intend to demonstrate that such a feature is not an exceptional occurrence in the idealised model of delta-interactions, but instead is structural and is present in any generic approximation of the model with a “physical” Hamiltonian with interactions of finite (i.e., non-zero) range around the points of the lattice \mathcal{Z}_κ .

In order to make this precise, let us recall quickly the spectral properties of $-\Delta_{\alpha_1, \alpha_2, \kappa}$.

Owing to the periodicity of the interaction, one can exploit the same Bloch–Floquet reduction scheme customarily used for Schrödinger operators with periodic potentials (see [20] Section XIII.16). Indeed the emerging picture, that we discuss briefly here below, is completely analogous to the classical one for continuous potentials. One introduces, for each $k \in (-\pi, \pi]$, the Hilbert space

$$\mathcal{H}_k = \{u \in L^2_{\text{loc}}(\mathbb{R}) \mid u(x + 1) = e^{ik} u(x) \text{ for a.e. } x \in \mathbb{R}\} \tag{1.5}$$

equipped with the scalar product

$$\langle u, v \rangle_{\mathcal{H}_k} = \int_0^1 \overline{u} v \, dx, \tag{1.6}$$

the corresponding direct integral with fibers \mathcal{H}_k , namely the Hilbert space $\int_{(-\pi, \pi]}^\oplus \mathcal{H}_k \frac{dk}{2\pi}$ of functions $k \mapsto u_k$ on $(-\pi, \pi]$ with values $u_k \in \mathcal{H}_k$ and with finite norm $\int_{(-\pi, \pi]} \|u_k\|_{\mathcal{H}_k}^2 \frac{dk}{2\pi}$, and the unitary map

$$\begin{aligned} U : L^2(\mathbb{R}) &\xrightarrow{\cong} \int_{(-\pi, \pi]}^\oplus \mathcal{H}_k \frac{dk}{2\pi} \\ (Uf)_k(x) &:= \sum_{n \in \mathbb{Z}} e^{ink} f(x - n). \end{aligned} \tag{1.7}$$

It is seen that by means of the isomorphism (1.7) the alternating KP Hamiltonian (1.3) is unitarily equivalent to

$$U(-\Delta_{\alpha_1, \alpha_2, \kappa})U^{-1} = \int_{(-\pi, \pi]}^{\oplus} (-\Delta_{\alpha_1, \alpha_2, \kappa}^{(k)}) \frac{dk}{2\pi} \quad (1.8)$$

where the fiber Hamiltonian $-\Delta_{\alpha_1, \alpha_2, \kappa}^{(k)}$ is the self-adjoint operator on \mathcal{H}_k given by

$$-\Delta_{\alpha_1, \alpha_2, \kappa}^{(k)} = -\frac{d^2}{dx^2} \quad (1.9)$$

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

The spectral properties of $-\Delta_{\alpha_1, \alpha_2, \kappa}$ are recovered from the spectral properties of each $-\Delta_{\alpha_1, \alpha_2, \kappa}^{(k)}$ via the decomposition (1.8). One finds (see, e.g., [24, Proposition 1]):

- Theorem 1.1** (i) $-\Delta_{\alpha_1, \alpha_2, \kappa}^{(k)}$ has purely discrete spectrum for each $k \in (-\pi, \pi]$.
(ii) $-\Delta_{\alpha_1, \alpha_2, \kappa}^{(k)}$ and $-\Delta_{\alpha_1, \alpha_2, \kappa}^{(-k)}$ are antiunitarily equivalent under ordinary complex conjugation, whence in particular their eigenvalues are identical and their eigenfunctions are complex conjugate.
(iii) Denoting by $E_\ell(k)$, $\ell = 1, 2, \dots$, the ℓ -th eigenvalue of $-\Delta_{\alpha_1, \alpha_2, \kappa}^{(k)}$ 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.
(iv) 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 $k = \pi$.
(v) The spectrum $\sigma(-\Delta_{\alpha_1, \alpha_2, \kappa})$ of $-\Delta_{\alpha_1, \alpha_2, \kappa}$ is purely absolutely continuous and has the structure

$$\sigma(-\Delta_{\alpha_1, \alpha_2, \kappa}) = \bigcup_{\ell=1}^{\infty} E_\ell([0, \pi]). \quad (1.10)$$

The interval $(-\pi, \pi]$ in which k ranges is the well-known Brillouin zone and (1.10) gives the familiar spectral structure of bands and gaps determined by the eigenvalues of the fiber Hamiltonian $-\Delta_{\alpha_1, \alpha_2, \kappa}^{(k)}$ at the centre ($k = 0$) and at the edge ($k = \pi$) of the Brillouin zone. Two consecutive spectral bands $E_\ell([0, \pi])$ and $E_{\ell+1}([0, \pi])$ are separated by a gap whenever

$$\begin{aligned} E_\ell(\pi) &< E_{\ell+1}(\pi) && \text{if } \ell \text{ is odd,} \\ E_\ell(0) &< E_{\ell+1}(0) && \text{if } \ell \text{ is even.} \end{aligned} \quad (1.11)$$

In the first case one says that the gap occurs at the edge of the Brillouin zone, in the second that it occurs at the centre of the Brillouin zone. The open interval

$$G_\ell := \begin{cases} (E_\ell(\pi), E_{\ell+1}(\pi)) & \text{if } \ell \text{ is odd} \\ (E_\ell(0), E_{\ell+1}(0)) & \text{if } \ell \text{ is even} \end{cases} \quad (1.12)$$

is the ℓ -th gap and the closed interval $E_\ell([0, \pi])$ is the ℓ -th band in the spectrum of $-\Delta_{\alpha_1, \alpha_2, \kappa}$. According to this numbering, (1.10) gives an alternation of bands and gaps. A gap can be possibly empty, in which case the gap is said to be vanishing and the two adjacent bands merge.

We underline once again that the above picture for the spectrum of periodic interactions of *zero range* is perfectly analogous to the well-known one for regular interactions of *finite range*, which we will be referring to in the following. The classical counterpart of Theorem 1.1 above for smooth potentials can be found, for instance, in Theorems XIII.89 and XIII.90 of [20].

In all cases, it is worth stressing that the presence of spectral gaps between bands of permitted energy has a crucial effect on the properties of conductance and insulation of the crystal that is modelled by a periodic interaction. There is vast literature concerned with the characterisation of vanishing and non-vanishing gaps for interactions of finite range, namely for classes of periodic potentials (see for instance, for the one-dimensional case, the overview given in Section 2 of [25]). The class of periodic point interactions has the advantage of allowing for exact, explicit computations of bands, gaps, and the associated transmission and reflection coefficients; the analysis for the Kronig–Penney model is completely worked out, for instance, in Section III.2.3 of [1].

Back to the model considered in this work, a complete characterisation of the bands and gaps of the spectrum of the generalised KP Hamiltonian for arbitrary values of the interaction strengths α_1, α_2 and of the lattice spacing κ was first obtained by Yoshitomi in [24]. The peculiar feature of the spectrum of the alternating KP Hamiltonian is that vanishing gaps are only possible for interaction strengths of opposite magnitude and for rational lattice spacing, in which case those gaps that remain open are determined by the lattice spacing itself. More precisely, the following holds:

Theorem 1.2 [24, Theorem 3] *Let $-\Delta_{\alpha_1, \alpha_2, \kappa}$ be the Hamiltonian defined in (1.3) for $\alpha_1 \neq \alpha_2$ and let G_ℓ , $\ell = 1, 2, \dots$, be the gaps in its spectrum, as defined in (1.12).*

- (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*

$$\begin{aligned} G_\ell &= \emptyset & \text{for } \ell \in 2n\mathbb{N}, \\ G_\ell &\neq \emptyset & \text{for } \ell \notin 2n\mathbb{N}. \end{aligned}$$

- (iii) *If $\alpha_2 = -\alpha_1$ and $2\kappa = m/n$ for two relatively prime integers $m, n \in \mathbb{N}$ such that m is even, then*

$$\begin{aligned} G_\ell &= \emptyset & \text{for } \ell \in n\mathbb{N}, \\ G_\ell &\neq \emptyset & \text{for } \ell \notin n\mathbb{N}. \end{aligned}$$

The case accounted for in part (i) of Theorem 1.2 above is the generic one. Actually, the fact that no spectral gap of the alternating KP Hamiltonian vanishes if κ is irrational and $\alpha_1 + \alpha_2 \neq 0$ is completely analogous to that occurring in the case of piecewise continuous periodic potentials, where it can be proven [14, 22] that the set of C^∞ , real-valued periodic potentials for which all gaps are non-zero is a dense G_δ -subset of the space $C^\infty(\mathbb{R})$ topologised with the semi-norms $\|f\|_n := \|\frac{d^n}{dx^n} f\|_\infty$, $n = 0, 1, 2, \dots$

On the opposite side, the case $\alpha_2 = -\alpha_1 =: \alpha$ and $\kappa = \frac{1}{2}$ (whence $\mathcal{Z}_\kappa = \frac{1}{2}\mathbb{Z}$), namely $n = m = 1$ in Theorem 1.2(ii), corresponds to the vanishing of all even gaps, namely all gaps at the centre of the Brillouin zone. It is this case that we intend to discuss further, focusing thus on the so-called *alternating* KP Hamiltonian $-\Delta_\alpha := -\Delta_{\alpha, -\alpha, \frac{1}{2}}$, i.e., the self-adjoint operator

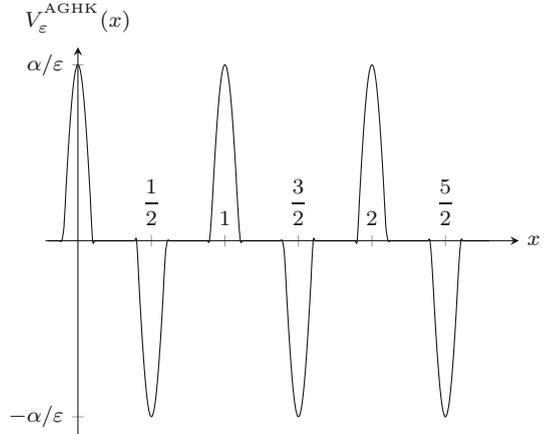
$$-\Delta_\alpha = -\frac{d^2}{dx^2} \quad \mathcal{D}(-\Delta_\alpha) = \left\{ \begin{array}{l} \psi \in H^2(\mathbb{R} \setminus \frac{1}{2}\mathbb{Z}) \cap H^1(\mathbb{R}) \\ \text{such that, } \forall n \in \mathbb{Z}, \\ \psi'(n^+) - \psi'(n^-) = \alpha\psi(n) \\ \psi'((n + \frac{1}{2})^+) - \psi'((n + \frac{1}{2})^-) = -\alpha\psi(n + \frac{1}{2}) \end{array} \right\}. \quad (1.13)$$

We are indeed in the condition now to state our problem:

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 the approximating “physical” model of alternating periodic interactions of finite (non-zero) range?

In other words we investigate whether such a peculiar spectral feature emerges only under the idealisation of a periodic interaction with alternating magnitude by means of delta-pseudo-potentials, or is instead already present in an actual periodic potential shaped as very peaked bumps with finite support. This would tell whether the alternating KP model (which, as already remarked, is a particularly effective idealisation in that it retains the main features of a periodic interaction and allows for explicit computations in terms of only one simple parameter α) reproduces a finite-range interaction phenomenon or it introduces a new spectral phenomenon, as far as the gap vanishing is concerned.

Incidentally, we remark that such a scenario is typical with point interactions. A paradigmatic example is the celebrated Thomas effect, namely the emergence of an infinity of negative energy eigenvalues accumulating to $-\infty$ for a three-body system: as long as the two-body interactions among particles have finite range the system is stable (i.e., the spectrum is bounded below), but when the interaction is assumed to have zero range then the Thomas effect occurs in a three-body system of identical bosons [17, 18] or also three different particles [15, 16] (but not two identical fermions and a third particle of different nature [5]). In such cases one has a spectral phenomenon that is typical only of the point interaction and has no counterpart for finite range interactions.

Fig. 1 The function $V_\varepsilon^{\text{AGHK}}$ 

It is worth commenting on why the problem stated above is non-trivial. A standard approximation of $-\Delta_\alpha$ in terms of Schrödinger Hamiltonians with finite-range periodic potentials, due to Albeverio et al. [2], is well-known; these potentials consist of a sequence of bumps, peaked at each integer or half-integer $n/2$, of the form

$$(-1)^n \frac{\alpha}{\varepsilon} V\left(\frac{x - n/2}{\varepsilon}\right)$$

for some $V \in L^1(\mathbb{R})$ such that $\int_{\mathbb{R}} V dx = 1$, and some $\varepsilon > 0$. The Schrödinger operator on $L^2(\mathbb{R})$ associated with the resulting “AGHK potential”

$$V_\varepsilon^{\text{AGHK}}(x) := \sum_{n \in \mathbb{Z}} (-1)^n \frac{\alpha}{\varepsilon} V\left(\frac{x - n/2}{\varepsilon}\right) \quad (1.14)$$

(see Fig. 1) is shown to converge, as $\varepsilon \rightarrow 0$, to $-\Delta_\alpha$ in the norm resolvent sense (see details also in [1, Theorem III.2.2.1], and in Sect. 3 of the present work). As well-known [23, Theorem 6.38], norm resolvent convergence prevents the spectrum of the approximants to suddenly contract or expand in the limit: more precisely

$$\lim_{\varepsilon \downarrow 0} \sigma\left(-\frac{d^2}{dx^2} + V_\varepsilon^{\text{AGHK}}\right) = \sigma(-\Delta_\alpha). \quad (1.15)$$

However this does *not* exclude that the gaps in $\sigma(-\frac{d^2}{dx^2} + V_\varepsilon^{\text{AGHK}})$ may stay open at any finite $\varepsilon > 0$ and only vanish in the limit.

In fact we shall see that this is precisely what happens, namely the spectral gaps of AGHK potential at the centre of the Brillouin zone are *not* all closed! In this respect, the AGHK approximant Hamiltonian and the limit KP Hamiltonian display a substantially different behaviour. Our problem consist of finding, if any, a better approximating potential.

A second motivation for our problem, based on the property (1.15), is that if one produces a smooth periodic potential that approximates the alternating KP delta-interactions in the norm resolvent sense and for which it is proved by other means that all the gaps at the centre of the Brillouin zone vanish, then it is possible to reproduce at once the vanishing of all such gaps also for $-\Delta_\alpha$, without embarking on the conceptually simple but practically tedious and lengthy analysis performed in [24] to prove Theorem 2.1 (a study of the zeroes of the discriminant of the corresponding ODE by means of the associated monodromy matrix and, in the end, of a system of algebraic equations). Indeed, if the gaps are already vanishing before the limit (1.15), so they remain in the limit.

In order to control the gaps of approximating smooth periodic potentials we shall make use of the work [25] by Michelangeli and Zagordi, in which a necessary and sufficient condition is discussed for the gaps at the centre of the Brillouin zone to vanish. This will allow us to answer our problem by engineering a suitable modification of the AGHK ‘bump’-like potential.

Let us then state our main results in a somewhat qualitative form, that will be formulated explicitly in Sect. 3 (Theorem 3.1).

Theorem 1.3 *For fixed $\alpha \in \mathbb{R}$ consider the alternating KP Hamiltonian $-\Delta_\alpha$ defined in (1.13). For each $\varepsilon > 0$ sufficiently small there exists a real-valued periodic potential $V_\varepsilon \in C(\mathbb{R})$, with unit period, such that the Hamiltonian $H_\varepsilon := -\frac{d^2}{dx^2} + V_\varepsilon$, defined on the domain of self-adjointness $H^2(\mathbb{R})$, converges to $-\Delta_\alpha$ as $\varepsilon \rightarrow 0$ in the norm resolvent sense, and all its gaps at the center of the Brillouin zone are closed.*

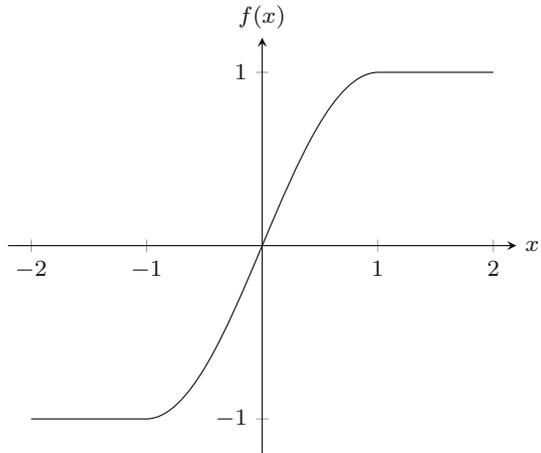
We find it instructive to re-state Theorem 1.3 in the following alternative form—that too will be proved in Sect. 3—which emphasises the fine tuning on the AGHK ‘bump’-like potential which is needed to obtain the desired convergence.

Theorem 1.4 *For fixed $\alpha \in \mathbb{R}$, consider the alternating KP Hamiltonian $-\Delta_\alpha$ defined in (1.13) and let $V_\varepsilon^{\text{AGHK}}$, $\varepsilon > 0$, be the corresponding AGHK ‘bump’-like potential (1.14) whose Schrödinger operator approximates $-\Delta_\alpha$ in the norm resolvent sense as $\varepsilon \rightarrow 0$. Then:*

- (i) $-\frac{d^2}{dx^2} + V_\varepsilon^{\text{AGHK}}$ converges to $-\Delta_\alpha$ in norm resolvent sense as $\varepsilon \rightarrow 0$, yet not all gaps at the centre of the Brillouin zone for the spectrum of $-\frac{d^2}{dx^2} + V_\varepsilon^{\text{AGHK}}$ vanish.
- (ii) *It is always possible to modify each bump of $V_\varepsilon^{\text{AGHK}}$ 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 $\tilde{V}_\varepsilon^{\text{AGHK}}$ has the following properties: for each ε , all the gaps at the centre of the Brillouin zone for the spectrum of $-\frac{d^2}{dx^2} + \tilde{V}_\varepsilon^{\text{AGHK}}$ vanish, and as $\varepsilon \rightarrow 0$ the operator $-\frac{d^2}{dx^2} + \tilde{V}_\varepsilon^{\text{AGHK}}$ too converges to $-\Delta_\alpha$ in the norm resolvent sense. $\tilde{V}_\varepsilon^{\text{AGHK}}$ here is precisely V_ε of Theorem 1.3.*

It is immediate to conclude from Theorems 1.3 or 1.4, together with the above mentioned well-known behaviour of the spectrum under norm resolvent convergence, our final answer to the problem stated initially:

Fig. 2 An example of an admissible function f



Corollary 1 *The gaps at the centre of the Brillouin zone for the spectrum of $-\Delta_\alpha$ vanish as well in a class of smooth periodic potentials that approximate $-\Delta_\alpha$ in the norm resolvent sense. This reproduces Theorem 1.2(ii) as far as the even gaps are concerned.*

We deduce from the previous theorems also a side result that is interesting in its own: let us cast it in the following remark. It concerns the *odd* gaps of the approximating Hamiltonians $-\frac{d^2}{dx^2} + V_\varepsilon^{\text{AGHK}}$ or $-\frac{d^2}{dx^2} + \tilde{V}_\varepsilon^{\text{AGHK}}$, i.e., those gaps at the edge ($k = \pi$) of the Brillouin zone.

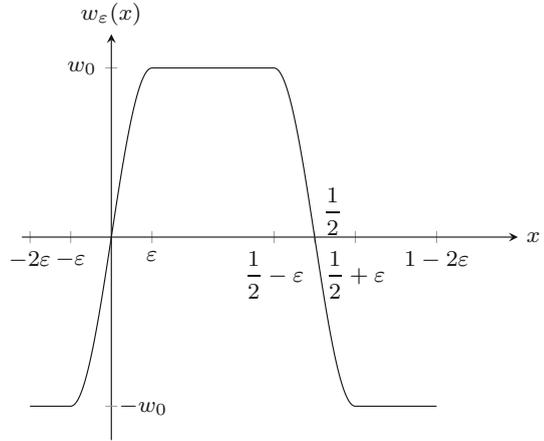
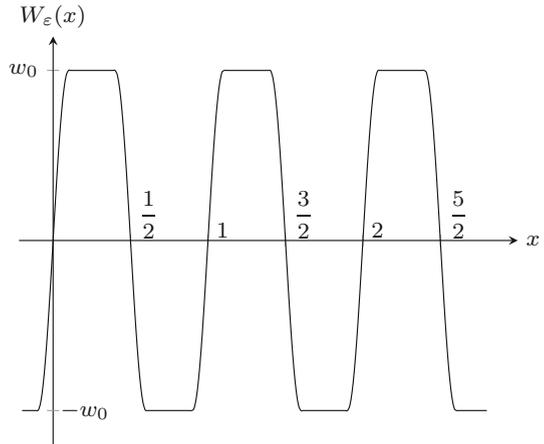
Remark 1 (Odd gaps for the approximating KP models)

- (i) Each odd gap $G_{2\ell+1}$ of $-\frac{d^2}{dx^2} + V_\varepsilon^{\text{AGHK}}$ or $-\frac{d^2}{dx^2} + \tilde{V}_\varepsilon^{\text{AGHK}}$ is open for $0 < \varepsilon < \varepsilon_\ell$, for some $\varepsilon_\ell > 0$ (however, there might not be uniformity in ε , meaning that possibly $\inf_\ell \varepsilon_\ell = 0$). Indeed $G_{2\ell+1}$ is open for the limit operator $-\Delta_\alpha$ (Theorem 1.2(ii)) and since the above two operators converge both to $-\Delta_\alpha$ in norm resolvent sense as $\varepsilon \rightarrow 0$ (Theorems 1.3, 1.4), their spectrum cannot suddenly expand in the limit.
- (ii) For fixed $\varepsilon > 0$, the spectrum of $-\frac{d^2}{dx^2} + \tilde{V}_\varepsilon^{\text{AGHK}}$ has infinitely many open odd gaps. For if not, then by standard properties of the spectrum of periodic Schrödinger operators [7, 8, 14] the potentials $V_\varepsilon^{\text{AGHK}}$ or $\tilde{V}_\varepsilon^{\text{AGHK}}$ should be necessarily *real analytic* functions, which is manifestly not the case (compare also to Fig. 5).

2 Approximating model with finite range interactions

In this section we introduce and discuss the potential V_ε of Theorem 1.3. In the following section we shall discuss the limit $\varepsilon \rightarrow 0$.

For each $\varepsilon \in (0, \frac{1}{4})$ we introduce a real-valued, continuous, periodic function V_ε , with period 1, as follows. Let $f \in C^1(\mathbb{R})$ be such that $f(x) \equiv -1$ for $x \leq -1$ and $f(x) \equiv 1$ for $x \geq 1$ (see, e.g., Fig. 2). For a fixed $w_0 \in \mathbb{R}$ we define (see Fig. 3)

Fig. 3 The function w_ε **Fig. 4** The function W_ε 

$$w_\varepsilon(x) := \begin{cases} w_0 f\left(\frac{x}{\varepsilon}\right) & \text{for } -2\varepsilon \leq x \leq 2\varepsilon, \\ w_0 & \text{for } 2\varepsilon \leq x \leq \frac{1}{2} - 2\varepsilon, \end{cases} \quad x \in \left[-2\varepsilon, \frac{1}{2} - 2\varepsilon\right], \quad (2.1)$$

$$w_\varepsilon(x) := -w_\varepsilon\left(x - \frac{1}{2}\right), \quad x \in \left[\frac{1}{2} - 2\varepsilon, 1 - 2\varepsilon\right].$$

Clearly $w_\varepsilon \in C^1([-2\varepsilon, 1 - 2\varepsilon])$. We extend it by periodicity to the whole real line by defining

$$W_\varepsilon(x) := w_\varepsilon(y) \quad \text{if } x = y + n \text{ for some } y \in [-2\varepsilon, 1 - 2\varepsilon] \text{ and } n \in \mathbb{Z}.$$

The fact that w_ε is constantly equal to $-w_0$ on $[-2\varepsilon, -\varepsilon] \cup [1/2 + \varepsilon, 1 - 2\varepsilon]$ guarantees that the function W_ε itself is of class C^1 (see Fig. 4). By construction W_ε

has period 1 and changes sign after each half-period, i.e.,

$$W_\varepsilon \left(x + \frac{1}{2} \right) = -W_\varepsilon(x) \quad \forall x \in \mathbb{R}. \quad (2.2)$$

In turn, we set

$$V_\varepsilon(x) := -w_0^2 + W_\varepsilon(x)^2 + W'_\varepsilon(x). \quad (2.3)$$

V_ε is thus a continuous, real-valued function with period 1. Owing to a standard Kato–Rellich argument [21, Theorem 8.8], the corresponding Schrödinger operator

$$\begin{aligned} H_\varepsilon &= -\frac{d^2}{dx^2} + V_\varepsilon \\ \mathcal{D}(H_\varepsilon) &= H^2(\mathbb{R}) \end{aligned} \quad (2.4)$$

is self-adjoint on the space $L^2(\mathbb{R})$. It therefore gives rise to a purely absolutely continuous spectrum with a typical structure in bands and gaps [20, Theorem XIII.90]. A first reason for the above choice of W_ε 's, and hence of V_ε 's, is that for such potentials *all* gaps of the spectrum of H_ε at the centre of the Brillouin zone are *closed*; conversely, any potential with closed gaps at the centre of the Brillouin zone must have the form (2.3) up to an additive constant. More precisely, the following is known:

Theorem 2.1 [25] *Let V be a continuous, real-valued potential with period 1. A necessary and sufficient condition for the spectrum of $-\frac{d^2}{dx^2} + V$ to have all gaps vanishing at the centre of the Brillouin zone is that*

$$V(x) = v_0 + W^2(x) + W'(x) \quad (2.5)$$

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

$$W \left(x + \frac{1}{2} \right) = -W(x) \quad \forall x \in \mathbb{R}. \quad (2.6)$$

If this is the case, then

$$W(x) = -\frac{1}{2} \int_x^{x+\frac{1}{2}} \left[V(y) - \int_0^1 V(t) dt \right] dy \quad (2.7)$$

and

$$v_0 = \int_0^1 [V(x) - W^2(x)] dx. \quad (2.8)$$

We remark that whereas here we are only using one implication of Theorem 2.1, in the proof of Theorem 1.4 we will need both implications.

The way V_ε is engineered is also to give it a specific shape of localised bumps which is well suited for the limit $\varepsilon \rightarrow 0$. More precisely (see Fig. 5), we see that by

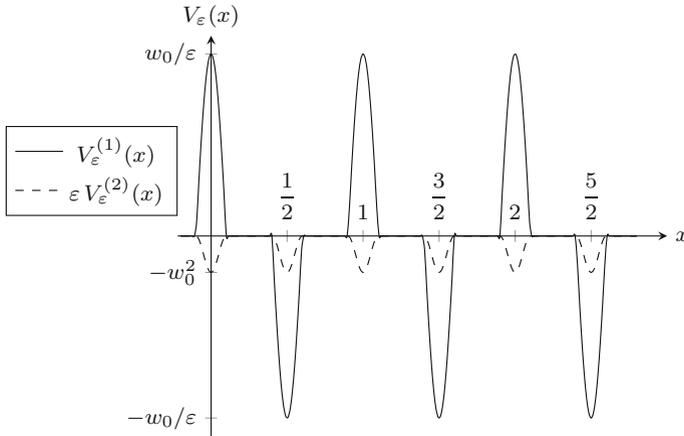


Fig. 5 The function $V_\varepsilon^{(1)}$ (continued line) and the function $\varepsilon V_\varepsilon^{(2)}$ (dashed line)

construction V_ε can be decomposed as

$$V_\varepsilon(x) = V_\varepsilon^{(1)}(x) + \varepsilon V_\varepsilon^{(2)}(x), \quad x \in \mathbb{R}, \quad (2.9)$$

where both $V_\varepsilon^{(1)}$ and $V_\varepsilon^{(2)}$ have a ‘bump’-like shape given by

$$V_\varepsilon^{(1)}(x) = \sum_{n \in \mathbb{Z}} U_{\varepsilon, n}^{(1)} \left(x - \frac{n}{2} \right), \quad (2.10)$$

and

$$V_\varepsilon^{(2)}(x) = \sum_{n \in \mathbb{Z}} U_\varepsilon^{(2)} \left(x - \frac{n}{2} \right), \quad (2.11)$$

the profile of each bump being given by

$$U_{\varepsilon, n}^{(1)}(x) := \frac{1}{\varepsilon} U_n^{(1)} \left(\frac{x}{\varepsilon} \right), \quad U_n^{(1)}(x) := (-1)^n w_0 f'(x), \quad (2.12)$$

and

$$U_\varepsilon^{(2)}(x) := \frac{1}{\varepsilon} U^{(2)} \left(\frac{x}{\varepsilon} \right), \quad U^{(2)}(x) := w_0^2 (f^2(x) - 1). \quad (2.13)$$

The ε -dependent bumps introduced above are peaked around each integer and half-integer, with a repeated profile given by (2.12) and (2.13) in terms of w_0 and f , supported on each interval $[\frac{n}{2} - \varepsilon, \frac{n}{2} + \varepsilon]$ of size 2ε , and with peak magnitude of order ε^{-1} . In particular the bumps in $V_\varepsilon^{(1)}$ point alternately upwards and downwards, the bumps in $V_\varepsilon^{(2)}$ have instead all the same direction.

Since the contribution of $V_\varepsilon^{(2)}$ in (2.9) is weighted by a factor ε , we have thus identified in V_ε a leading profile of alternating bumps whose peaks are of order ε^{-1} and a sub-leading profile consisting of bumps of order 1 in ε .

It is clear already at this stage that as $\varepsilon \rightarrow 0$ the bump-like potential $V_\varepsilon^{(1)}$ mimics better and better an alternating Kronig–Penney delta-potential, as we shall discuss more rigorously in the next section, whereas the remainder potential $\varepsilon V_\varepsilon^{(2)}$ is expected to become negligible in the limit—its support shrinks to a set of isolated points with integer and half-integer coordinate, while the peaks remain uniformly bounded.

On the other hand the remainder term $\varepsilon V_\varepsilon^{(2)}$, albeit not relevant in the limit, is crucial at every non-zero ε in order to ensure that the spectral gaps at the centre of the Brillouin zone for the periodic potential V_ε are all closed. Indeed, as we have already commented, it is the sum (2.9), and not its first summand only, that satisfies Theorem 2.1 (compare the proof of Theorem 1.4 in Sect. 3).

Remark 2 The constant term in the definition (2.3) of V_ε , namely $-w_0^2$, could also be set to an arbitrary value $v_{\varepsilon,0} \in \mathbb{R}$, and the statement of Theorem 2.1 would still hold. However, we performed the choice $V_{\varepsilon,0} \equiv -w_0^2$ because then the decomposition (2.9) avoids having a non-zero constant term.

3 Convergence to the alternating KP Hamiltonian

In this section we prove the convergence results we stated in the Introduction. With the notation of the previous section, we are now in the condition of re-formulating and proving Theorem 1.3 in the following explicit form:

Theorem 3.1 *Let $\alpha \in \mathbb{R}$ and, correspondingly, let $-\Delta_\alpha$ be the alternating KP Hamiltonian (1.13) with interaction strength α . Moreover, let H_ε , $\varepsilon \in (0, \frac{1}{4})$, be the Hamiltonian defined through (2.1), (2.3), and (2.4) with coupling constant $w_0 := \frac{1}{2}\alpha$. Then $H_\varepsilon \rightarrow -\Delta_\alpha$ in norm resolvent sense as $\varepsilon \rightarrow 0$.*

Proof We introduce the operator

$$H_\varepsilon^{\text{AGHK}} := -\frac{d^2}{dx^2} + V_\varepsilon^{(1)}, \quad \mathcal{D}(H_\varepsilon^{\text{AGHK}}) = H^2(\mathbb{R}) \tag{3.1}$$

on $L^2(\mathbb{R})$, which is self-adjoint because of the same Kato–Rellich argument used for H_ε . One observes that $-\Delta_\alpha$, H_ε , and $H_\varepsilon^{\text{AGHK}}$, for all ε 's, are uniformly bounded below and have the same form domain $H^1(\mathbb{R})$, where the quadratic form of $-\Delta_\alpha$ (see (1.4)) is

$$(-\Delta_\alpha)[\varphi, \psi] = \int_{\mathbb{R}} \overline{\varphi'} \psi' dx + \alpha \sum_{n \in \mathbb{Z}} (-1)^n \overline{\varphi\left(\frac{n}{2}\right)} \psi\left(\frac{n}{2}\right) \tag{3.2}$$

and, for convenience, we split the quadratic form of H_ε as

$$H_\varepsilon[\varphi, \psi] = H_\varepsilon^{\text{AGHK}}[\varphi, \psi] + \varepsilon V_\varepsilon^{(2)}[\varphi, \psi]. \tag{3.3}$$

Owing to this particular occurrence, by standard properties of the norm resolvent convergence [19, Theorem VIII.25(c)] we see that, in order to prove that $H_\varepsilon \rightarrow -\Delta_\alpha$

in norm resolvent sense as $\varepsilon \rightarrow 0$, it is enough to prove

$$\sup_{\substack{\varphi \in H^1(\mathbb{R}) \setminus \{0\} \\ \psi \in H^1(\mathbb{R}) \setminus \{0\}}} \frac{|H_\varepsilon[\varphi, \psi] - (-\Delta_\alpha)[\varphi, \psi]|}{\|\varphi\|_{H^1} \|\psi\|_{H^1}} \xrightarrow{\varepsilon \downarrow 0} 0. \quad (3.4)$$

Moreover, we recognise that

$$\sup_{\substack{\varphi \in H^1(\mathbb{R}) \setminus \{0\} \\ \psi \in H^1(\mathbb{R}) \setminus \{0\}}} \frac{|H_\varepsilon^{\text{AGHK}}[\varphi, \psi] - (-\Delta_\alpha)[\varphi, \psi]|}{\|\varphi\|_{H^1} \|\psi\|_{H^1}} \xrightarrow{\varepsilon \downarrow 0} 0. \quad (3.5)$$

Indeed, the discussion done in Sect. 2 shows that the periodic potential $V_\varepsilon^{(1)}$ has a bump-like structure, see (2.10) and (2.12), that satisfies the assumptions of Theorem III.2.2.1 in [1], namely the above-mentioned result by Albeverio, Gesztesy, Høegh-Krohn, and Kirsch that establishes

$$H_\varepsilon^{\text{AGHK}} \xrightarrow{\varepsilon \downarrow 0} -\Delta_\alpha \quad \text{in norm resolvent sense} \quad (3.6)$$

precisely by proving (3.5) (which is (III.2.2.20) in [1]). In particular, it is the choice we made for f in (2.1) and for $w_0 = \frac{1}{2}\alpha$ that guarantees that the KP Hamiltonian emerging in the limit has the correct interaction strengths: these are given, according to (III.2.2.9) in [1] and (2.10)–(2.12) above, by

$$\int_{\mathbb{R}} U_n^{(1)}(x) dx = \int_{\mathbb{R}} (-1)^n w_0 f'(x) dx = (-1)^n 2w_0 = (-1)^n \alpha, \quad n \in \mathbb{Z},$$

reproducing precisely the alternating interaction strengths of $-\Delta_\alpha$. Therefore, it only remains to prove

$$\sup_{\substack{\varphi \in H^1(\mathbb{R}) \setminus \{0\} \\ \psi \in H^1(\mathbb{R}) \setminus \{0\}}} \frac{|\varepsilon V_\varepsilon^{(2)}[\varphi, \psi]|}{\|\varphi\|_{H^1} \|\psi\|_{H^1}} \xrightarrow{\varepsilon \downarrow 0} 0 \quad (3.7)$$

because the conclusion (3.4) will then follow from (3.3), (3.5), and (3.7). To this aim, we find

$$\begin{aligned} |V_\varepsilon^{(2)}[\varphi, \psi]| &= \left| \int_{\mathbb{R}} V_\varepsilon^{(2)} \overline{\varphi} \psi dx \right| \\ &= \left| \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}} \frac{1}{\varepsilon} U^{(2)} \left(\frac{x - n/2}{\varepsilon} \right) \overline{\varphi(x)} \psi(x) dx \right| \\ &= \left| \sum_{n \in \mathbb{Z}} \int_{\frac{n}{2} - \varepsilon}^{\frac{n}{2} + \varepsilon} \frac{1}{\varepsilon} U^{(2)} \left(\frac{x - n/2}{\varepsilon} \right) \overline{\varphi(x)} \psi(x) dx \right| \\ &\leq \sum_{n \in \mathbb{Z}} \|\varphi\|_{L^\infty[\frac{n}{2} - \varepsilon, \frac{n}{2} + \varepsilon]} \|\psi\|_{L^\infty[\frac{n}{2} - \varepsilon, \frac{n}{2} + \varepsilon]} \left| \int_{-1}^1 U^{(2)}(y) dy \right| \end{aligned} \quad (3.8)$$

$$\begin{aligned} &\leq c \sum_{n \in \mathbb{Z}} \|\varphi\|_{H^1(\frac{n}{2}-\varepsilon, \frac{n}{2}+\varepsilon)} \|\psi\|_{H^1(\frac{n}{2}-\varepsilon, \frac{n}{2}+\varepsilon)} \\ &\leq c \|\varphi\|_{H^1(\mathbb{R})} \|\psi\|_{H^1(\mathbb{R})} \end{aligned}$$

uniformly for $\varepsilon \in (0, \frac{1}{4})$, where we used (2.11) and (2.13) in the second step, the fact that $\text{supp}(U^{(2)}) = [-1, 1]$ in the third step, a standard Sobolev embedding in the fifth step, and the Schwarz inequality in the last step. Clearly (3.8) implies (3.7) and the proof is thus completed.

Concerning Theorem 1.4, we can now specify the potentials mentioned in the statement, namely the AGHK potential and its modification, that in terms of the potentials constructed in Sect. 2 are expressed by

$$\begin{aligned} V_\varepsilon^{\text{AGHK}} &:= V_\varepsilon^{(1)}, \\ \tilde{V}_\varepsilon^{\text{AGHK}} &:= V_\varepsilon^{(1)} + \varepsilon V_\varepsilon^{(2)} = V_\varepsilon. \end{aligned} \tag{3.9}$$

Our notation $V_\varepsilon^{\text{AGHK}}$ for the potential $V_\varepsilon^{(1)}$ defined in (2.10) and (2.12) is to stress that this is the ‘‘canonical’’ (continuous) periodic potential, which one introduces in the canonical approximation of the alternating KP delta-pseudo-potential à-la Albeverio, Gesztesy, Høegh-Krohn, and Kirsch (Theorem III.2.2.1 in [1]), consisting of alternating bumps peaked around each period and half-period, each of which spikes up as $\varepsilon \rightarrow 0$ to a delta-like profile with strength given by the integral of the bump. (In that construction $V_\varepsilon^{\text{AGHK}}$ can be also chosen in a slightly more general manner than here, allowing each bump to have a different profile, as long as all such profiles are uniformly bounded by a $L^1(\mathbb{R})$ -function and scale with ε in the appropriate way.)

Proof (Proof of Theorem 1.4) Let the AGHK periodic potential that approximates at the scale $\varepsilon > 0$ the alternating KP delta-pseudo-potential with strength $\alpha \in \mathbb{R}$ be given by (1.14) for some ‘bump’-like profile V that is continuous, with support in $[-1, 1]$, and such that $\int_{\mathbb{R}} V dx = 1$:

$$V_\varepsilon^{\text{AGHK}}(x) = \sum_{n \in \mathbb{Z}} (-1)^n \frac{\alpha}{\varepsilon} V\left(\frac{x - n/2}{\varepsilon}\right). \tag{3.10}$$

The convergence of $-\frac{d^2}{dx^2} + V_\varepsilon^{\text{AGHK}}$ to $-\Delta_\alpha$ in norm resolvent sense as $\varepsilon \rightarrow 0$ is the standard result (3.6) [2].

We observe that such $V_\varepsilon^{\text{AGHK}}$ cannot be of the form (2.5) for a C^1 -function $W_\varepsilon^{\text{AGHK}}$ that satisfies (2.6). Indeed, if this was the case, namely if

$$V_\varepsilon^{\text{AGHK}}(x) = v_{\varepsilon,0}^{\text{AGHK}} + W_\varepsilon^{\text{AGHK}}(x)^2 + \frac{d}{dx} W_\varepsilon^{\text{AGHK}}(x) \tag{3.11}$$

for some constant $v_{\varepsilon,0}^{\text{AGHK}}$, then $W_\varepsilon^{\text{AGHK}}$ would be prescribed by (2.7), that is,

$$\frac{d}{dx} W_\varepsilon^{\text{AGHK}}(x) = \frac{1}{2}(V_\varepsilon^{\text{AGHK}}(x) - V_\varepsilon^{\text{AGHK}}(x + 1/2)) \tag{3.12}$$

(indeed $\int_0^1 V_\varepsilon dx = 0$). Since by construction (3.10) satisfies $V_\varepsilon^{\text{AGHK}}(x + \frac{1}{2}) = -V_\varepsilon^{\text{AGHK}}(x)$, (3.12) above reads

$$\frac{d}{dx} W_\varepsilon^{\text{AGHK}}(x) = V_\varepsilon^{\text{AGHK}}(x). \quad (3.13)$$

Plugging (3.13) into (3.11) yields $(W_\varepsilon^{\text{AGHK}})^2 \equiv -v_{\varepsilon,0}^{\text{AGHK}}$, hence $W_\varepsilon^{\text{AGHK}}$ is constant, being a $C^1(\mathbb{R})$ -function. In view of (3.13), this would imply $V_\varepsilon^{\text{AGHK}} \equiv 0$, a contradiction.

On the other hand, it is immediately seen that $V_\varepsilon^{\text{AGHK}}$ takes the form of $V_\varepsilon^{(1)}$ of (2.10) and (2.12) as long as one sets

$$f(x) := -1 + 2 \int_{-\infty}^x V dy, \quad w_0 := \frac{\alpha}{2}. \quad (3.14)$$

Indeed f is a $C^1(\mathbb{R})$ -function such that $f \equiv -1$ for $x \leq -1$, $f \equiv 1$ for $x \geq 1$, and $f' = 2V$.

In turn, if one defines $V_\varepsilon^{(2)}$ by (2.11) and (2.13) in terms of such f and w_0 and, correspondingly, $\tilde{V}_\varepsilon^{\text{AGHK}}$ as the sum $V_\varepsilon^{(1)} + \varepsilon V_\varepsilon^{(2)}$, one concludes the following:

- since f has the properties used in the construction of Sect. 2, the potential $\tilde{V}_\varepsilon^{\text{AGHK}}$ can be re-written in the form (2.3) and hence is in the class of those periodic potentials described by Theorem 2.1 for which $-\frac{d^2}{dx^2} + \tilde{V}_\varepsilon^{\text{AGHK}}$ has all gaps vanishing at the centre of the Brillouin zone;
- since instead $V_\varepsilon^{\text{AGHK}}$ has not the form (2.5), the reverse implication of Theorem 2.1 prescribes that some of the even gaps of $-\frac{d^2}{dx^2} + V_\varepsilon^{\text{AGHK}}$ must remain open.

This completes the proof of part (i) of the Theorem, as well as of the first statement of part (ii). The second statement of part (ii) is precisely Theorem 3.1 above.

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