



HAL
open science

Integrated density of states: from the finite range to the periodic Airy-Schroedinger operator

Hakim Boumaza, Olivier Lafitte

► **To cite this version:**

Hakim Boumaza, Olivier Lafitte. Integrated density of states: from the finite range to the periodic Airy-Schroedinger operator. 2020. hal-02964056

HAL Id: hal-02964056

<https://hal.science/hal-02964056>

Preprint submitted on 14 Oct 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

INTEGRATED DENSITY OF STATES: FROM THE FINITE RANGE TO THE PERIODIC AIRY-SCHRÖDINGER OPERATOR

H. BOUMAZA AND O. LAFITTE

ABSTRACT. We compute an explicit formula for the integrated density of states of the periodic Airy-Schrödinger operator on the real line. The potential of this Schrödinger operator is periodic, continuous and piecewise affine. For this purpose, we study precisely the spectrum of the Schrödinger operator whose potential is the restriction of the periodic Airy-Schrödinger potential to a finite number of periods. We prove that all the eigenvalues of the operator corresponding to the restricted potential are in the spectral bands of the periodic Airy-Schrödinger operator and none of them are in its spectral gaps. We count exactly the number of these eigenvalues in each of these spectral bands. Note that our results depend on a semiclassical parameter and are valid for values of it larger than explicit constants.

1. THE MODEL AND MAIN RESULTS

In [2], we obtained the band spectrum of the Airy-Schrödinger operator $-\hbar^2 \frac{d^2}{dx^2} + V$ where V is periodic of period 2, even, continuous, piecewise affine with maximum value 0 and minimal value some reference potential $-V_0$ with $V_0 \in \mathbb{R}_+^*$. However, from our analysis, the question of what could be, physically, the contribution to the behavior of the scattered solution for each value of an energy in a band is not obtained by the classical method of bands analysis. Instead of this, we consider (as Fermi's Golden rule says) the infinite system as a limit of a finite system where the results should not be dependent on the length of the box.

We study the integrated density of states (IDS for short) of the periodic Airy-Schrödinger operator whose definition is recalled at (4). The IDS is a function of the real variable which counts the number of proper energy states below a fixed energy E . This number corresponds to the maximal number of electrons of energy smaller than E since, by Pauli's exclusion principle, two electrons cannot be in the same proper energy state. Since the periodic Airy-Schrödinger has a band spectrum and no eigenvalue, one cannot directly define such a function. To avoid this issue, the IDS is defined as a thermodynamical limit (see Definition 1). The existence of this limit is proven alongside the computation of its explicit value in the proof of Theorem 2. The definition of the IDS of the periodic Airy-Schrödinger involves the restriction of this operator to a finite (odd) number of periods. It leads us to introduce the multiple wells Airy-Schrödinger operator as in Section 1.1. The eigenfunctions of this operator are the wave functions describing the electronic transport in a potential which is made of $2N + 1$ triangular wells. We prove that this operator has exactly $2N + 2$ eigenvalues in each spectral band of the periodic Airy-Schrödinger operator and no eigenvalues in the spectral gaps.

Most of the results for the IDS of periodic Schrödinger operators in dimension 1 and higher are known for potentials which are at least of class C^2 at their minima points (see [6, 7, 13, 17]). All these results are asymptotics of the IDS for large energies. Our first motivation, from a mathematical point of view, is to get the analog of these results in the case of a potential which is not regular at its minima (and maxima) points. We also compare

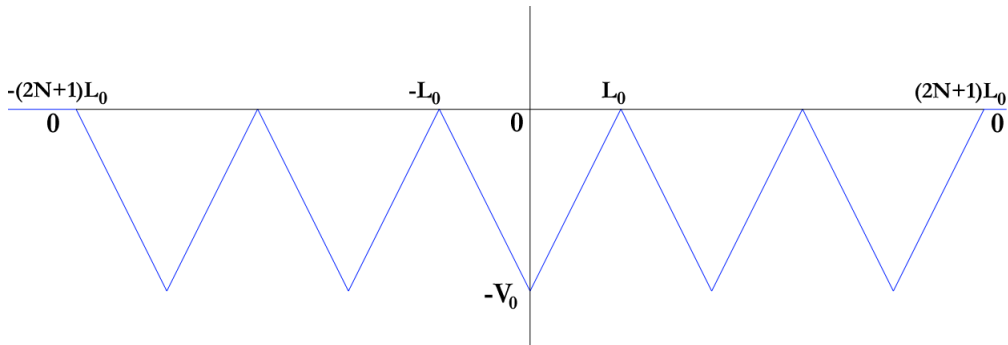


FIGURE 1. The potential V_{2N+1} for $N = 2$.

our results to the asymptotics of the IDS obtained for singular potentials such as random potentials as in, for example, the Kronig-Penney model (see [10]). We discuss these topics in Section 1.2.

If one wants to study the physics corresponding to the Integrated Density of States (IDS) in the physics of photonics crystals as well as the physics of semi-conductors, the relevant quantity is what is called the density of states (DOS) (as one can observe from Kar (figure 1.3) [8] which recalls the classical expression for the parabolic density of states, expressed through $E - E_c = \frac{k^2 \hbar^2}{2m^*}$, in the 0d to 3d cases). It describes the probability density measure of electrons in a conduction band and of holes (places being able to accept electrons) in a valence band (which are the first and second band of the problem of concern in our paper). It appears, as the name suggests, that the IDS is the repartition function of the DOS. Apart from very few exact cases, the DOS is observed and measured for experimental devices ([8], [19]), or computed using the Bloch functions of the problem (called classically the orbitals of the atom) [4]. More precisely, one considers a finite but large number of Bloch modes to compute numerically the eigenvalues of the operator with the associated compactly supported potential (as in the present paper), showing approximations of the DOS (fig. 5, fig. 6). Note for example that Yang and al [19] characterize the inorganic semiconductors with a parabolic DOS, and the organic ones with a Gaussian DOS (fig. 2).

In all these cases of the Physics community, the potential giving rise to the Bloch modes is seldom exhibited, and the relevant function studied in nearly all the papers is the DOS, which describes the density of the eigenvalues. An exact expression of the IDS hence of the DOS it thus a really interesting mathematical as well as physical result.

The periodic triangular potential of the multiple wells Airy-Schrödinger operator appears in some physical models as, for example, [12] in which the authors claim that they are able to study the spectrum of Schrödinger operators with general piecewise-linear potentials. Their approach was already to use transfer matrices but they did only compute numerically the eigenenergies for some particular piecewise-linear potentials (and thus fail to obtain precise asymptotic results). They also compare these numerics with numerical computations for the WKB approximation. Hence, beside our interest in the IDS of the periodic Airy-Schrödinger operator, another motivation for studying the spectrum of the multiple wells Airy-Schrödinger operator is to give a complete mathematical treatment of one example of Schrödinger operator with piecewise-linear potential. Our results for the multiple wells Airy-Schrödinger model could give a mathematical counterpart to the numerical results obtained by physicists.

1.1. The multiple wells Airy-Schrödinger operator. Let $N \geq 0$ be an integer and let $2L_0 \in \mathbb{R}_+^*$ be a characteristic length modelling the distance between two ions in a one dimensional finite lattice of $2N + 1$ ions. The motion of electrons in this finite lattice can be studied through the following Schrödinger operator acting on the subspace of the Sobolev space $H^2(\mathbb{R})$,

$$D(H_{2N+1}) = \{\psi \in H^2(\mathbb{R}) \mid \psi(-(2N+1)L_0) = \psi((2N+1)L_0)\}$$

by

$$H_{2N+1} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_{2N+1}, \quad (1)$$

where \hbar is the reduced Planck constant, m the mass of an electron and V_{2N+1} is the multiplication operator by :

$$V_{2N+1} : x \mapsto \sum_{k=-N}^N V(x - 2kL_0) \quad (2)$$

where $V : \mathbb{R} \rightarrow \mathbb{R}$ is defined by

$$V(x) = \begin{cases} V_0 \left(\frac{|x|}{L_0} - 1 \right) & \text{if } x \in [-L_0, L_0] \\ 0 & \text{elsewhere} \end{cases}, \quad (3)$$

$V_0 \in \mathbb{R}_+^*$ being a reference potential. The potential V_{2N+1} is continuous on \mathbb{R} and continuously differentiable everywhere except at its minima and maxima points. Note that V_{2N+1} is an even function.

We recall the definition of the periodic Airy-Schrödinger operator as defined in [2]. Let

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \tilde{V}, \quad (4)$$

where \tilde{V} is the $2L_0$ -periodic function equal to V on $[-L_0, L_0]$. The description of the spectrum of H is already given in [2] but for reader's convenience, let us recall it here. The operator H has purely absolutely continuous spectrum and this spectrum is a union of closed intervals (see [15, XIII]):

$$\sigma(H) = \bigcup_{p \geq 0} [E_{\min}^p, E_{\max}^p]. \quad (5)$$

For $p \geq 0$, $[E_{\min}^p, E_{\max}^p]$ is called the p -th spectral band, $(E_{\max}^p, E_{\min}^{p+1})$ the p -th spectral gap and E_{\min}^p and E_{\max}^p are called the spectral band edges. The band edges are characterized through the theory of Bloch decomposition for periodic Schrödinger operators. More precisely, let $\omega \in [-L_0, L_0]$. Consider the restriction $H(\omega)$ of H to $H^2([-L_0, L_0])$, the Sobolev space of functions $\psi \in H^2(\mathbb{R})$ which satisfy

$$\psi(L_0) = e^{i(\frac{\pi}{L_0}\omega + \pi)}\psi(-L_0) \quad \text{and} \quad \psi'(L_0) = e^{i(\frac{\pi}{L_0}\omega + \pi)}\psi'(-L_0). \quad (6)$$

The operator $H(\omega)$ is self-adjoint, Hilbert-Schmidt and thus compact. Its spectrum consists only on isolated eigenvalues and we set

$$\sigma(H(-L_0)) := \{E_{\min}^0, E_{\max}^1, E_{\min}^2, E_{\max}^3, \dots\} \quad \text{and} \quad \sigma(H(0)) := \{E_{\max}^0, E_{\min}^1, E_{\max}^2, E_{\min}^3, \dots\}.$$

In order to describe the spectrum of the operator H_{2N+1} , one considers the equation:

$$H_{2N+1}\psi = E\psi, \quad E \in \mathbb{R}, \quad \psi \in D(H_{2N+1}). \quad (7)$$

After rescaling and translating, this equation is equivalent to an Airy equation on each interval $]kL_0, (k+1)L_0[$, for $k \in \{-(2N+1), \dots, 2N\}$. Thus we introduce u and v , the canonical solutions of the Airy equation, satisfying

$$u(0) = 1, \quad u'(0) = 0 \quad \text{and} \quad v(0) = 0, \quad v'(0) = 1.$$

In particular, the Wronskian of u and v , $uv' - u'v$, is constant and equal to 1. Both u and v are analytic functions on \mathbb{R} . Moreover, u and v are strictly increasing and positive on $(0, +\infty)$. Thus, the zeroes of u , v and their derivatives are all real numbers in $(-\infty, 0]$.

Notation. We denote by $\{-c_{2j+1}\}_{j \geq 0} \cup \{0\}$ and $\{-c_{2j}\}_{j \geq 0}$ the set of the zeroes of respectively v and v' arranged in decreasing order.

Notation. Let

$$c = \left(\frac{2mL_0^2 V_0}{\hbar^2} \right)^{\frac{1}{3}}. \quad (8)$$

As we will see in (12), this parameter corresponds to the height of the potential barrier. It will play the role of a semiclassical parameter and the semiclassical limit reads c tends to $+\infty$.

We now state the first result of this article which describe the spectrum of H_{2N+1} and compare it to the spectrum of the periodic Airy-Schrödinger operator in the range of the potential, the interval $[-V_0, 0]$.

Theorem 1. (1) *The spectrum of H_{2N+1} is equal to its point spectrum and*

$$\sigma(H_{2N+1}) \cap [-V_0, 0] \subset \sigma(H) \cap [-V_0, 0]. \quad (9)$$

(2) *For each p in \mathbb{N} , for every $c \geq c_p$ and every $i \in \{0, \dots, p\}$,*

$$\#(\sigma(H_{2N+1}) \cap [E_{\min}^i, E_{\max}^i]) = 2N + 2. \quad (10)$$

Hence all the eigenvalues of H_{2N+1} are in the band spectrum of H . In particular there is no eigenvalue of H_{2N+1} in the interior of the spectral gaps of H . Recall also that from [2, Theorem 2.4], all the spectral bands $[E_{\min}^i, E_{\max}^i]$ in (10) are included in the interval $[-V_0, 0]$. These results remain true for an even number of wells as explained in Appendix C.

As the results of [2] for the periodic Airy-Schrödinger operator, Theorem 1 is not stated in the semiclassical limit, but for the semiclassical parameter c larger than an explicit constant. More precisely, one can have access to p bands in a very precise way when $c \geq c_p$. Observe that the needed estimates become much more difficult to prove when c is close to c_p than when c can be taken arbitrarily large (see Proof of Lemma 1 in Appendix B).

For general results in the semiclassical limit for multiple wells with singularities at their minima, we refer to [18]. These results apply to H_{2N+1} . But, in our example, we are able to have more precise results on the counting of the eigenvalues and, as said before, our results are not only valid in the semiclassical limit but for values of the semiclassical parameter larger than explicit constants, for which we can control a finite number of bands. This was made possible because (7) leads to an equation in E which is solvable with classical special functions, independent on the semiclassical parameter.

Theorem 1 also gives an example for general results such as [5, Proposition 2.9]. In our case, we prove a precise count of the eigenvalues in the spectral bands of the corresponding periodic operator and the absence of eigenvalues embedded in the spectral gaps. To be more precise, as the hypothesis of [5] do not hold for H_{2N+1} , we can only say that our results are consistent with the general picture described in [5].

1.2. The IDS of the periodic Airy-Schrödinger operator. The IDS of H is the distribution function of its energy levels per unit volume. A way to define it properly is to restrict the operator H to finite length intervals and consider a thermodynamical limit. Since the definition of the domain of H_{2N+1} includes Dirichlet boundary conditions at $\pm(2N+1)L_0$, one can take the following definition for the IDS associated to H .

Definition 1. *The IDS associated to H is the function from \mathbb{R} to \mathbb{R}_+ , $E \mapsto I(E)$, where $I(E)$, for $E \in \mathbb{R}$, is defined by*

$$I(E) = \lim_{N \rightarrow +\infty} \frac{1}{2(2N+1)L_0} \#\{\lambda \leq E; \lambda \in \sigma(H_{2N+1})\}. \quad (11)$$

For the existence of this limit and general properties of the IDS, we refer to the textbooks [3, 9].

To determine the expression of the IDS of H , we localize more precisely the eigenvalues of H_{2N+1} . To solve equation (7) we rescale it by setting $\mathbf{E} = c\frac{E}{V_0}$ and defining \mathbf{V}_{2N+1} , the multiplication operator by the rescaled potential $\mathbf{V}_{2N+1} : z \mapsto \sum_{k=-N}^N \mathbf{V}(z-2k)$ where

$$\mathbf{V}(z) = \begin{cases} |z| - 1 & \text{if } z \in [-1, 1] \\ 0 & \text{elsewhere} \end{cases}.$$

We also set, for every $p \geq 0$, $\mathbf{E}_{\min}^p = c\frac{E_{\min}^p}{V_0}$ and $\mathbf{E}_{\max}^p = c\frac{E_{\max}^p}{V_0}$. With $x = L_0z$ in (7), this equation is equivalent to

$$\begin{aligned} \mathbf{H}_{2N+1}\phi &:= -\frac{d^2}{dz^2}\phi + c^3\mathbf{V}_{2N+1}\phi = c^2\mathbf{E}\phi, \quad \mathbf{E} \in \mathbb{R}, \\ \phi &\in H^2(\mathbb{R}), \quad \phi(-2N+1) = \phi(2N+1). \end{aligned} \quad (12)$$

which defines the rescaled operator \mathbf{H}_{2N+1} . One similarly defines the rescaled periodic Airy-Schrödinger operator \mathbf{H} whose spectral bands are the intervals $[\mathbf{E}_{\min}^p, \mathbf{E}_{\max}^p]$.

As \mathbf{V}_{2N+1} is continuous and bounded, any solution ϕ of (12) is continuously differentiable on \mathbb{R} .

In the sequel, we will restrict ourselves to energies \mathbf{E} in the range of $c\mathbf{V}_{2N+1}$, the interval $[-c, 0]$.

To give the expression of the IDS of \mathbf{H} we need to introduce more notations. Let $\mathbf{E} \in [-c, 0]$. We denote by \mathbf{U} and \mathbf{V} the functions defined, for every $x \in \mathbb{R}$, by

$$\mathbf{U}(x) = v'(-c - \mathbf{E})u(x) - u'(-c - \mathbf{E})v(x) \quad (13)$$

and

$$\mathbf{V}(x) = u(-c - \mathbf{E})v(x) - v(-c - \mathbf{E})u(x). \quad (14)$$

In particular, the Wronskian of \mathbf{U} and \mathbf{V} is equal to 1. These functions \mathbf{U} and \mathbf{V} appear in the equations characterizing the spectral band edges of \mathbf{H} ([2, (3.18)-(3.21)]) and are also called the Bloch modes of the operator \mathbf{H}_{2N+1} . Indeed, the spectral band edges of \mathbf{H} are exactly the zeroes of \mathbf{U} , \mathbf{V} and their derivatives. Hence, the sign of $\mathbf{U}\mathbf{U}'\mathbf{V}\mathbf{V}'$ changes exactly at each spectral band edge and it justifies the introduction of the following function:

$$\varphi : \begin{cases} \sigma(\mathbf{H}) & \rightarrow [0, \pi] \\ \mathbf{E} & \mapsto \text{Arg}((\mathbf{U}'\mathbf{V} + \mathbf{U}\mathbf{V}' + 2i\sqrt{-\mathbf{U}\mathbf{U}'\mathbf{V}\mathbf{V}'})(-\mathbf{E})) \end{cases} \quad (15)$$

where for any complex number $a + ib$, $\text{Arg}(a + ib)$ denotes its argument. We also denote by φ the extension of the function φ to \mathbb{R} which maps any value outside of $\sigma(\mathbf{H})$ to 0. The value 0 of this extension is coherent with the signs of $\mathbf{U}\mathbf{V}'$ and $\mathbf{U}'\mathbf{V}$ in the spectral bands and gaps as given in Section 3.1.

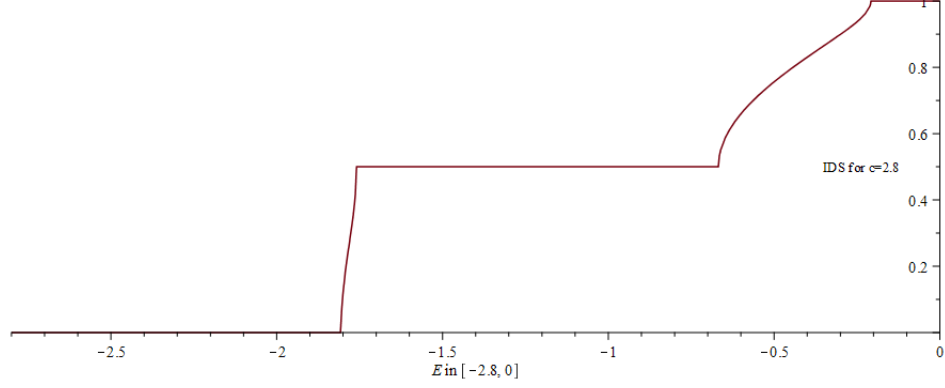


FIGURE 2. The IDS on $[-c, 0]$ for $c = 2.8$. The two first spectral bands appear.

Remark that the complex number which appears in the argument in (15) is of modulus 1 (see (61)). Hence, using the signs of UV' and $U'V$ in the spectral bands as given in Section 3.1, we get a simplified expression of φ :

$$\forall \mathbf{E} \in \sigma(\mathbf{H}), \varphi(\mathbf{E}) = 2\text{Arctan} \left(\sqrt{\frac{-U'V}{UV'}} \right) (-\mathbf{E}). \quad (16)$$

From (16), one deduces that in the neighborhood of each spectral band edge, the function φ has a squareroot behavior. We precise this, prove (16) and give a heuristic approximation of $\varphi(\mathbf{E})$ in the interior of the spectral bands in Appendix A.

Denote the integer part of a real number x by $[x]$ and the characteristic function of an interval $[c, d]$ by $\mathbf{1}_{[c,d]}$.

Theorem 2. *Assume that $c \geq c_0$. For any $\mathbf{E} \in [-c, 0]$, the integrated density of states associated to \mathbf{H} is given by*

$$\mathbf{I}(\mathbf{E}) = \frac{1}{2}p(\mathbf{E}) + \begin{cases} \frac{1}{2\pi}\varphi(\mathbf{E}) \cdot \mathbf{1}_{[E_{\min}^{p(\mathbf{E})}, E_{\max}^{p(\mathbf{E})}]}(\mathbf{E}) & \text{if } p(\mathbf{E}) \text{ is even} \\ \left(\frac{1}{2} - \frac{1}{2\pi}\varphi(\mathbf{E})\right) \cdot \mathbf{1}_{[E_{\min}^{p(\mathbf{E})}, E_{\max}^{p(\mathbf{E})}]}(\mathbf{E}) & \text{if } p(\mathbf{E}) \text{ is odd} \end{cases} \quad (17)$$

where $p(\mathbf{E})$ is the smallest integer such that $\mathbf{E} \leq \mathbf{E}_{\max}^{p(\mathbf{E})}$ and is given by

$$p(\mathbf{E}) = \left\lceil \frac{4}{3\pi}(c + \mathbf{E})^{\frac{3}{2}} \right\rceil. \quad (18)$$

In particular, we remark that the function $\mathbf{E} \mapsto \mathbf{I}(\mathbf{E})$ is continuous on the interval $[-c, 0]$. In the proof of Proposition 1, we give an explicit formula for φ in terms of functions \mathbf{U} and \mathbf{V} (see (62), (63) and (64)). Also note that the factor $\frac{1}{2}$ in the formulae (17) is the inverse of the length of one period of the potential \mathbf{V} .

The formula (17) is the analog, for the continuous periodic Airy-Schrödinger operator, of the formula of the IDS in [14] for a discrete periodic Schrödinger operator.

The asymptotic behavior of \mathbf{I} for c and $-\mathbf{E}$ large is different than the one given by the results of [16] as presented in [17], for a smooth C^∞ potential. They lead to an IDS with an asymptotic in $E^{\frac{1}{2}}$ for E large, different from our case which leads to an asymptotic proportional to $(-\mathbf{E})^{\frac{3}{2}}$. The non C^1 regularity at the minima points of the potential leads

to a different behavior than in the regular case. In dimension larger than 1, the same differences for the asymptotic behavior are to be found in other papers like [6], [7] or [13] where the potential (or periodic perturbation in [6]) has regularity properties stronger than in our setting.

The results of [6, 7, 13, 17] on the IDS are stated for general periodic potentials with some regularity assumption (in [7] it is given through its Fourier coefficients). It leads to precise asymptotics in energy for the IDS. The results for multiple wells in [18] are given for a general C^2 potential which is C^3 in a neighborhood of some non-critical energy and leads to estimates on the IDS of the corresponding Schrödinger operator in the semiclassical limit. Here, since we look at a particular example of periodic operator for which the eigenvalues equations are explicitly solvable, we have been able not only to find the asymptotics of the IDS as in [6, 7, 13, 17] or an estimate as in [18], but an explicit formula for it.

In the case of a potential which is not at least C^2 , we refer again to [18]. In particular, the result of Theorem 2 is compatible with the lower bounds and upper bounds found in [18, Propositions 6.6 and 6.7]. Note that the results of [18] are stated in the semiclassical limit, hence for a “large enough” semiclassical parameter. No explicit lower bound for the semiclassical parameter gives the validity domain of [18, Propositions 6.6 and 6.7], compared to Theorem 2 which states that the given formula is valid for every c larger than the constant c_0 . Note that c_0 is explicitly known as a zero of a classical function.

Another interesting case of singular potential is the case of random potentials like the Anderson model in dimension 1 or the Kronig-Penney model. In this case, we refer to the results of [10] where an asymptotic in $\frac{\sqrt{E}}{\pi}$ for E large is given for the IDS. This asymptotic is equal, up to a factor 2 equal to the period of the potential, to the derivative of the asymptotic $\frac{4}{3\pi}E^{\frac{3}{2}}$ of the IDS of the periodic Airy-Schrödinger operator. We note that the weak second derivative of the potential \mathbf{V} is equal to the Kronig-Penney potential with constant non-random coefficients equal to ± 2 . This gives an illustration of the results [11, Theorem 4.1 and Theorem 6.2C] which, through the m -functions of Weyl and Titchmarsh and the w function of Kotani, link the IDS and the potential. The derivative, with respect to the energy, of the IDS associated to the potential \mathbf{V} compares to the IDS associated to the weak second derivative of \mathbf{V} .

2. THE SPECTRUM OF \mathbf{H}_{2N+1}

2.1. Characterization of the eigenvalues of \mathbf{H}_{2N+1} . We start by characterizing the real numbers \mathbf{E} in $[-c, 0]$ such that (12) has a solution $\phi \in H^2(\mathbb{R})$ which is not identically equal to zero and such that $\phi(-(2N+1)) = \phi(2N+1)$.

From the canonical solutions u and v of the Airy equation, one defines the canonical pair of odd and even solutions of (12) on the interval $[-1, 1]$. The functions defined for every $z \in [-1, 1]$ by

$$U_{\text{even}}(z) = \mathbf{U}(c\mathbf{V}_{2N+1}(z) - \mathbf{E})$$

and

$$V_{\text{odd}}(z) = \text{sign}(z)\mathbf{V}(c\mathbf{V}_{2N+1}(z) - \mathbf{E})$$

form a basis of even and odd C^1 solutions of the equation (12) on the interval $[-1, 1]$. Indeed, one checks that U_{even} and V_{odd} are locally in the Sobolev space $H^2(\mathbb{R})$, thus are in $C^1(\mathbb{R})$. Their wronskian satisfies

$$\forall z \in [-1, 1], (U_{\text{even}}V'_{\text{odd}} - U'_{\text{even}}V_{\text{odd}})(z) = c.$$

In any interval of the form $[2n-1, 2n+1]$ for $n \in \{-N, \dots, N\}$, a solution ϕ of (12) writes

$$\forall z \in [2n-1, 2n+1], \phi(z) = A_n U_{\text{even}}(z-2n) + B_n V_{\text{odd}}(z-2n) \quad (19)$$

where A_n and B_n are real numbers. Note that $U_{\text{even}}(\pm(2N+1)) = \mathbf{U}(-\mathbf{E})$ and $V_{\text{odd}}(\pm(2N+1)) = \pm\mathbf{V}(-\mathbf{E})$. Hence, continuity of the solution ϕ and of its derivative at $2n+1$ for $n \in \{-N+1, \dots, N-1\}$ yields

$$A_n \mathbf{U}(-\mathbf{E}) + B_n \mathbf{V}(-\mathbf{E}) = A_{n+1} \mathbf{U}(-\mathbf{E}) - B_{n+1} \mathbf{V}(-\mathbf{E}) \quad (20)$$

$$c(A_n \mathbf{U}'(-\mathbf{E}) + B_n \mathbf{V}'(-\mathbf{E})) = -c(A_{n+1} \mathbf{U}'(-\mathbf{E}) - B_{n+1} \mathbf{V}'(-\mathbf{E})) \quad (21)$$

The minus sign in front of B_{n+1} in both (20) and (21) comes from the oddness of V_{odd} . One deduces from (20) and (21) that for every $n \in \{-N+1, \dots, N-1\}$,

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = \begin{pmatrix} (\mathbf{U}\mathbf{V}' + \mathbf{U}'\mathbf{V})(-\mathbf{E}) & 2(\mathbf{V}\mathbf{V}')(-\mathbf{E}) \\ 2(\mathbf{U}\mathbf{U}')(-\mathbf{E}) & (\mathbf{U}\mathbf{V}' + \mathbf{U}'\mathbf{V})(-\mathbf{E}) \end{pmatrix} \begin{pmatrix} A_n \\ B_n \end{pmatrix}. \quad (22)$$

using that the Wronskian of \mathbf{U} and \mathbf{V} is constant and equal to 1.

Notations. We set

$$a := (\mathbf{U}\mathbf{V}' + \mathbf{U}'\mathbf{V})(-\mathbf{E}), \quad (23)$$

$$b_0 := \begin{cases} \sqrt{(\mathbf{U}\mathbf{U}')(-\mathbf{E})} & \text{if } (\mathbf{U}\mathbf{U}')(-\mathbf{E}) > 0 \\ i\sqrt{(-\mathbf{U}\mathbf{U}')(-\mathbf{E})} & \text{if } (\mathbf{U}\mathbf{U}')(-\mathbf{E}) \leq 0 \end{cases} \quad (24)$$

$$b_1 := \begin{cases} \sqrt{(\mathbf{V}\mathbf{V}')(-\mathbf{E})} & \text{if } (\mathbf{V}\mathbf{V}')(-\mathbf{E}) > 0 \\ i\sqrt{(-\mathbf{V}\mathbf{V}')(-\mathbf{E})} & \text{if } (\mathbf{V}\mathbf{V}')(-\mathbf{E}) \leq 0. \end{cases} \quad (25)$$

We introduce the transfer matrix which maps the solution of (12) and its derivative on the interval $[2n-1, 2n+1]$ to the solution and its derivative on the interval $[2n+1, 2n+3]$:

$$T_{\mathbf{E}} := \begin{pmatrix} a & 2b_1^2 \\ 2b_0^2 & a \end{pmatrix}. \quad (26)$$

In particular we have

$$\begin{pmatrix} A_N \\ B_N \end{pmatrix} = T_{\mathbf{E}}^{2N+1} \begin{pmatrix} A_{-N} \\ B_{-N} \end{pmatrix}. \quad (27)$$

Now we turn to the C^1 conditions at $-(2N+1)$ and $2N+1$. On the interval $[2N+1, +\infty)$, the potential \mathbf{V}_{2N+1} is identically zero, thus, since ϕ is in particular in $L^2(\mathbb{R})$, one has

$$\forall z \in [2N+1, +\infty), \phi(z) = \phi(2N+1)e^{-\lambda(z-(2N+1))} \quad (28)$$

with λ a positive real number such that

$$-\lambda^2 = c^2 \mathbf{E}.$$

Without loss of generality one can choose ϕ such that $\phi(2N+1) = 1$. Indeed, ϕ is not identically equal to zero and $(\phi(2N+1), \phi'(2N+1)) = \phi(2N+1) \cdot (1, -\lambda)$. Hence by the Cauchy-Lipschitz theorem, $\phi(2N+1) \neq 0$. Then, since $\phi'(2N+1) = -\lambda$, one has

$$A_N \mathbf{U}(-\mathbf{E}) + B_N \mathbf{V}(-\mathbf{E}) = 1 \quad (29)$$

$$c(A_N \mathbf{U}'(-\mathbf{E}) + B_N \mathbf{V}'(-\mathbf{E})) = -\lambda. \quad (30)$$

Similarly, on the interval $(-\infty, -(2N+1)]$, one has

$$\forall z \in (-\infty, -(2N+1)], \phi(z) = \phi(-(2N+1))e^{\lambda(z+2N+1)} \quad (31)$$

with the same λ as in (28). Since $\phi(-(2N+1)) = \phi(2N+1) = 1$, one has

$$A_{-N} \mathbf{U}(-\mathbf{E}) - B_{-N} \mathbf{V}(-\mathbf{E}) = 1 \quad (32)$$

$$c(A_{-N} \mathbf{U}'(-\mathbf{E}) - B_{-N} \mathbf{V}'(-\mathbf{E})) = \lambda. \quad (33)$$

Solving the system formed by the equations (32) and (33) one deduces that

$$A_{-N} = \lambda \frac{1}{c^2} \mathbf{V}(-\mathbf{E}) + \frac{1}{c} \mathbf{V}'(-\mathbf{E}) \quad \text{and} \quad B_{-N} = \lambda \frac{1}{c^2} \mathbf{U}(-\mathbf{E}) + \frac{1}{c} \mathbf{U}'(-\mathbf{E}). \quad (34)$$

Combining (29) and (30),

$$\lambda(A_N \mathbf{U}(-\mathbf{E}) + B_N \mathbf{V}(-\mathbf{E})) = -c(A_N \mathbf{U}'(-\mathbf{E}) + B_N \mathbf{V}'(-\mathbf{E})). \quad (35)$$

We also remark that, since λ is positive, $\frac{\lambda}{c} = (-\mathbf{E})^{\frac{1}{2}}$. It leads to introduce the following function defined for $y \in [-c, 0]$ by:

$$\Phi(y) = (y+c)^{\frac{1}{2}}(A_N \mathbf{U}(y+c) + B_N \mathbf{V}(y+c)) + A_N \mathbf{U}'(y+c) + B_N \mathbf{V}'(y+c)$$

Then, (35) is equivalent to the equation in \mathbf{E} , $\Phi(-c - \mathbf{E}) = 0$. The change of variables $y = -c - \mathbf{E}$ leads us to introduce for any $p \geq 0$,

$$Y_{\min}^p = -c - \mathbf{E}_{\min}^p \quad \text{and} \quad Y_{\max}^p = -c - \mathbf{E}_{\max}^p.$$

Remark that $\mathbf{E} \in [\mathbf{E}_{\min}^p, \mathbf{E}_{\max}^p]$ if and only if $y \in [Y_{\max}^p, Y_{\min}^p]$. Hence, in the sequel, spectral bands or spectral gaps will refer indifferently to the intervals in the variable \mathbf{E} or y .

3. PROOF OF THEOREM 1

3.1. Preliminary : the signs of \mathbf{U} , \mathbf{U}' , \mathbf{V} , \mathbf{V}' . From the results of [2, Section 3.2], the spectral band edges are exactly the zeroes of these four functions. Let us be more precise. Assume that $j \geq 1$ is an integer:

- (1) The function $y \mapsto \mathbf{U}(y+c)$ vanishes at Y_{\max}^{4j+2} , is strictly negative on the interval $(Y_{\max}^{4j+2}, Y_{\max}^{4j})$, vanishes at Y_{\max}^{4j} and is strictly positive on $(Y_{\max}^{4j}, Y_{\max}^{4j-2})$.
- (2) The function $y \mapsto \mathbf{U}'(y+c)$ vanishes at Y_{\min}^{4j+2} , is strictly negative on the interval $(Y_{\min}^{4j+2}, Y_{\min}^{4j})$, vanishes at Y_{\min}^{4j} and is strictly positive on $(Y_{\min}^{4j}, Y_{\min}^{4j-2})$.
- (3) The function $y \mapsto \mathbf{V}(y+c)$ vanishes at Y_{\max}^{4j+1} , is strictly positive on the interval $(Y_{\max}^{4j+1}, Y_{\max}^{4j-1})$, vanishes at Y_{\max}^{4j-1} and is strictly negative on $(Y_{\max}^{4j-1}, Y_{\max}^{4j-3})$.
- (4) The function $y \mapsto \mathbf{V}'(y+c)$ vanishes at Y_{\min}^{4j+1} , is strictly positive on the interval $(Y_{\min}^{4j+1}, Y_{\min}^{4j-1})$, vanishes at Y_{\min}^{4j-1} and is strictly negative on $(Y_{\min}^{4j-1}, Y_{\min}^{4j-3})$.

| y | Y_{\max}^{4j+2} | Y_{\min}^{4j+2} | Y_{\max}^{4j+1} | Y_{\min}^{4j+1} | Y_{\max}^{4j} | Y_{\min}^{4j} | Y_{\max}^{4j-1} | Y_{\min}^{4j-1} | Y_{\max}^{4j-2} | Y_{\min}^{4j-2} | Y_{\max}^{4j-3} | Y_{\min}^{4j-3} | | | |
|---------------|-------------------|-------------------|-------------------|-------------------|-----------------|-----------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|---|---|---|
| band or gap | band | gap | band | gap | band | gap | band | gap | band | gap | band | | | | |
| \mathbf{U} | 0 | - | - | - | - | 0 | + | + | + | + | 0 | - | - | - | |
| \mathbf{U}' | | + | 0 | - | - | - | 0 | + | + | + | + | 0 | - | - | |
| \mathbf{V} | | | - | - | 0 | + | + | + | + | 0 | - | - | - | 0 | + |
| \mathbf{V}' | | | | | - | - | - | 0 | + | + | + | + | 0 | - | 0 |

TABLE 1. Signs of \mathbf{U} , \mathbf{U}' , \mathbf{V} , \mathbf{V}' on the interval $[Y_{\max}^{4j+2}, Y_{\min}^{4j-3}]$ for $j \geq 1$.

3.2. Expression of Φ . We have to compute the coefficients A_N and B_N to get the explicit expression of Φ . Thus we have to compute the matrix $T_{\mathbf{E}}^{2N+1}$. It suffices to diagonalize $T_{\mathbf{E}}$. For this, it is easier to separate the cases when \mathbf{E} is in a spectral gap of \mathbf{H} , \mathbf{E} is in an even spectral band (for an index p even) of \mathbf{H} and when \mathbf{E} is in an odd spectral band (for an index p odd) of \mathbf{H} .

3.2.1. *In the spectral gaps.* For \mathbf{E} in a spectral gap, $(\mathbf{U}\mathbf{U}')(-\mathbf{E}) > 0$ and $(\mathbf{V}\mathbf{V}')(-\mathbf{E}) > 0$. Thus, the eigenvalues of $T_{\mathbf{E}}$ are

$$a + 2b_0b_1 \text{ and } a - 2b_0b_1 \quad (36)$$

and the associated eigenvectors are

$$\begin{pmatrix} b_1 \\ b_0 \end{pmatrix} \text{ and } \begin{pmatrix} -b_1 \\ b_0 \end{pmatrix}. \quad (37)$$

We set

$$b := 2\sqrt{(\mathbf{U}\mathbf{U}'\mathbf{V}\mathbf{V}')(-\mathbf{E})} = 2b_0b_1. \quad (38)$$

We note that, for any \mathbf{E} in a spectral gap, $2\sqrt{(\mathbf{U}\mathbf{U}'\mathbf{V}\mathbf{V}')(-\mathbf{E})} < |(\mathbf{U}\mathbf{V}' + \mathbf{U}'\mathbf{V})(-\mathbf{E})|$. Indeed, if $2\sqrt{(\mathbf{U}\mathbf{U}'\mathbf{V}\mathbf{V}')(-\mathbf{E})} = |(\mathbf{U}\mathbf{V}' + \mathbf{U}'\mathbf{V})(-\mathbf{E})|$ then $((\mathbf{U}\mathbf{V}')(-\mathbf{E}) - (\mathbf{U}'\mathbf{V})(-\mathbf{E}))^2 = 0$ but $\mathbf{U}\mathbf{V}' - \mathbf{U}'\mathbf{V}$ is constant and equal to 1 since the Wronskian of u and v is equal to 1. Thus,

$$0 < b < |a|. \quad (39)$$

Then

$$T_{\mathbf{E}}^{2N+1} = \frac{1}{2^{2N+1}} \begin{pmatrix} b_1 & -b_1 \\ b_0 & b_0 \end{pmatrix} \begin{pmatrix} (a+b)^{2N+1} & 0 \\ 0 & (a-b)^{2N+1} \end{pmatrix} \begin{pmatrix} \frac{1}{b_1} & \frac{1}{b_0} \\ -\frac{1}{b_1} & \frac{1}{b_0} \end{pmatrix}.$$

This gives the expressions of the coefficients A_N and B_N and thus the expression of $\Phi(y)$ for y such that $-\mathbf{E}$ is in a gap of \mathbf{H} and $y \in [-c, 0]$:

$$\begin{aligned} \Phi(y) &= \frac{1}{2^{2N}} \left[((\mathbf{U}' + (\cdot)^{\frac{1}{2}}\mathbf{U})(\mathbf{V}' + (\cdot)^{\frac{1}{2}}\mathbf{V}))(y+c) \times ((a+b)^{2N+1} + (a-b)^{2N+1}) \right. \\ &\quad \left. + \left(\frac{b_1}{b_0}(\mathbf{U}' + (\cdot)^{\frac{1}{2}}\mathbf{U})^2 + \frac{b_0}{b_1}(\mathbf{V}' + (\cdot)^{\frac{1}{2}}\mathbf{V})^2 \right) (y+c) \times ((a+b)^{2N+1} - (a-b)^{2N+1}) \right] \quad (40) \end{aligned}$$

3.2.2. *In the interior of even spectral bands.* For $\mathbf{E} \in (\mathbf{E}_{\min}^{2j}, \mathbf{E}_{\max}^{2j})$, we have $(\mathbf{U}\mathbf{U}')(-\mathbf{E}) < 0$ and $(\mathbf{V}\mathbf{V}')(-\mathbf{E}) > 0$. Thus, the eigenvalues of $T_{\mathbf{E}}$ are

$$a + 2i\sqrt{-(\mathbf{U}\mathbf{U}'\mathbf{V}\mathbf{V}')(-\mathbf{E})} \text{ and } a - 2i\sqrt{-(\mathbf{U}\mathbf{U}'\mathbf{V}\mathbf{V}')(-\mathbf{E})}, \quad (41)$$

and the associated eigenvectors are

$$\begin{pmatrix} b_1 \\ b_0 \end{pmatrix} \text{ and } \begin{pmatrix} b_1 \\ -b_0 \end{pmatrix} \quad (42)$$

with $b_0 = i\sqrt{-(\mathbf{U}\mathbf{U}')(-\mathbf{E})}$ in this case. Assume that y is such that $-\mathbf{E}$ is in an even spectral band of \mathbf{H} and $y \in [-c, 0]$. We slightly change the previous notation of b in order to highlight the complex number i in the following expressions and we set

$$b(y+c) := 2\sqrt{-(\mathbf{U}\mathbf{U}'\mathbf{V}\mathbf{V}')(y+c)}. \quad (43)$$

We also set

$$\alpha(y+c) := \left(\sqrt{\frac{\mathbf{V}\mathbf{V}'}{-\mathbf{U}\mathbf{U}'}}(\mathbf{U}' + (\cdot)^{\frac{1}{2}}\mathbf{U})^2 \right) (y+c) \text{ and } \beta(y+c) := \left(\sqrt{\frac{-\mathbf{U}\mathbf{U}'}{\mathbf{V}\mathbf{V}'}}(\mathbf{V}' + (\cdot)^{\frac{1}{2}}\mathbf{V})^2 \right) (y+c) \quad (44)$$

Then, the expression of $\Phi(y)$ is:

$$\begin{aligned}
\Phi(y) &= \frac{1}{2^{2N+1}} \left[2((U' + (\cdot)^{\frac{1}{2}}U)(V' + (\cdot)^{\frac{1}{2}}V))(y+c) \times ((a+ib)^{2N+1} + (a-ib)^{2N+1})(y+c) \right. \\
&\quad \left. + (i\alpha - i\beta)(y+c) \times ((a+ib)^{2N+1} - (a-ib)^{2N+1})(y+c) \right] \\
&= \frac{1}{2^{2N+1}} ((a+ib)^{2N+1} + (a-ib)^{2N+1})(y+c) \left[2((U' + (\cdot)^{\frac{1}{2}}U)(V' + (\cdot)^{\frac{1}{2}}V))(y+c) \right. \\
&\quad \left. + (\alpha - \beta)(y+c) \times \tan((2N+1)\text{Arg}(a+ib)(y+c)) \right] \\
&= \frac{1}{2^{2N+1}} ((a+ib)^{2N+1} + (a-ib)^{2N+1})(y+c) \times (\alpha + \beta)(y+c) \\
&\quad \times \left[\left(\frac{2(U' + (\cdot)^{\frac{1}{2}}U)(V' + (\cdot)^{\frac{1}{2}}V)}{\alpha + \beta} \right) + \left(\frac{\alpha - \beta}{\alpha + \beta} \right) \times \tan((2N+1)\text{Arg}(a+ib)) \right] (y+c). \tag{45}
\end{aligned}$$

We also used that

$$\sqrt{\left(2(U' + (\cdot)^{\frac{1}{2}}U)(V' + (\cdot)^{\frac{1}{2}}V) \right)^2 + (\alpha - \beta)^2} = \alpha + \beta. \tag{46}$$

Let us introduce the function $k : \sigma(\mathbf{H}) \cap [-c, 0] \rightarrow \mathbb{R}$ define by

$$\forall y \in \sigma(\mathbf{H}) \cap [-c, 0], \quad k(y) = \left(\sqrt{-\frac{\mathbf{V}\mathbf{V}'}{\mathbf{U}\mathbf{U}'}} \times \frac{U' + (\cdot)^{\frac{1}{2}}U}{V' + (\cdot)^{\frac{1}{2}}V} \right) (y+c). \tag{47}$$

Then, (45) rewrites, for y such that $-\mathbf{E}$ is in an even spectral band of \mathbf{H} and $y \in [-c, 0]$ and since $\beta(y+c) > 0$:

$$\begin{aligned}
\Phi(y) &= \frac{1}{2^{2N+1}} ((a+ib)^{2N+1} + (a-ib)^{2N+1})(y+c) \times (\alpha + \beta)(y+c) \\
&\quad \times \left[\frac{2k(y)}{1 + (k(y))^2} + \frac{(k(y))^2 - 1}{(k(y))^2 + 1} \times \tan((2N+1)\text{Arg}(a+ib)(y+c)) \right]. \tag{48}
\end{aligned}$$

3.2.3. *In the interior of odd spectral bands.* For $\mathbf{E} \in (\mathbf{E}_{\min}^{2j+1}, \mathbf{E}_{\max}^{2j+1})$, we have $(\mathbf{U}\mathbf{U}')(-\mathbf{E}) > 0$ and $(\mathbf{V}\mathbf{V}')(-\mathbf{E}) < 0$. The eigenvalues of $T_{\mathbf{E}}$ are again

$$a + ib \text{ and } a - ib \tag{49}$$

and the associated eigenvectors are

$$\begin{pmatrix} b_1 \\ b_0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} -b_1 \\ b_0 \end{pmatrix} \tag{50}$$

with $b_1 = i\sqrt{-(\mathbf{V}\mathbf{V}')(-\mathbf{E})}$ in this case.

The expression of $\Phi(y)$ is, for y such that $-\mathbf{E}$ is in an odd spectral band of \mathbf{H} and $y \in [-c, 0]$:

$$\begin{aligned}
\Phi(y) &= \frac{1}{2^{2N+1}} ((a+ib)^{2N+1} + (a-ib)^{2N+1})(y+c) \times (\alpha + \beta)(y+c) \\
&\quad \times \left[\frac{2\tilde{k}(y)}{1 + (\tilde{k}(y))^2} + \frac{(\tilde{k}(y))^2 - 1}{(\tilde{k}(y))^2 + 1} \times \tan((2N+1)\text{Arg}(a+ib)(y+c)) \right]. \tag{51}
\end{aligned}$$

setting for $y \in \sigma(\mathbf{H}) \cap [-c, 0]$, $\tilde{k}(y) = \frac{1}{k(y)}$, since $k(y)$ does not vanish in the interior of the odd spectral bands.

3.3. **Counting the zeroes of Φ in $[-c, 0]$.** In this section, we prove that Φ does not vanish in the spectral gaps and has $2N + 2$ zeroes in each spectral band contained in $[-c, 0]$.

3.3.1. *In the spectral gaps.* Let $j \geq 1$ be an integer. From the signs of U , U' , V and V' given in Section 3.1, the function $y \mapsto U'(y+c) + (y+c)^{\frac{1}{2}}U(y+c)$ is strictly positive in the spectral gap $(Y_{\min}^{4j+3}, Y_{\max}^{4j+2})$, strictly negative in the spectral gaps $(Y_{\min}^{4j+2}, Y_{\max}^{4j+1})$ and $(Y_{\min}^{4j+1}, Y_{\max}^{4j})$ and strictly positive in the spectral gap $(Y_{\min}^{4j}, Y_{\max}^{4j-1})$.

The function $y \mapsto V'(y+c) + (y+c)^{\frac{1}{2}}V(y+c)$ is strictly negative in the spectral gaps $(Y_{\min}^{4j+3}, Y_{\max}^{4j+2})$ and $(Y_{\min}^{4j+2}, Y_{\max}^{4j+1})$, and strictly positive in the spectral gaps $(Y_{\min}^{4j+1}, Y_{\max}^{4j})$ and $(Y_{\min}^{4j}, Y_{\max}^{4j-1})$.

First case. Assume that we are in the spectral gap $(Y_{\min}^{4j+2}, Y_{\max}^{4j+1})$ or in the spectral gap $(Y_{\min}^{4j}, Y_{\max}^{4j-1})$. Then the product $(U'(y+c) + (y+c)^{\frac{1}{2}}U(y+c))(V'(y+c) + (y+c)^{\frac{1}{2}}V(y+c))$ is strictly positive and the functions $y \mapsto (UV')(y+c)$ and $y \mapsto (U'V)(y+c)$ are also strictly positive. Thus, $a > 0$, $b > 0$, $a+b > 0$ and, using (39), $a-b > 0$. Moreover, since $b > 0$, we always have $a+b > a-b$. According to the expression (40), $\Phi(y) > 0$ in the spectral gaps $(Y_{\min}^{4j+2}, Y_{\max}^{4j+1})$ and $(Y_{\min}^{4j}, Y_{\max}^{4j-1})$ hence does not vanish in these intervals.

Second case. Assume that we are in the spectral gap $(Y_{\min}^{4j+3}, Y_{\max}^{4j+2})$ or in the spectral gap $(Y_{\min}^{4j+1}, Y_{\max}^{4j})$. Then the product $(U'(y+c) + (y+c)^{\frac{1}{2}}U(y+c))(V'(y+c) + (y+c)^{\frac{1}{2}}V(y+c))$ is strictly negative and the functions $y \mapsto (UV')(y+c)$ and $y \mapsto (U'V)(y+c)$ are also strictly negative. Thus, $a < 0$, $b > 0$, and using (39), $a-b < 0$ and $a+b < 0$. Since $2N+1$ is odd, $(a+b)^{2N+1} < 0$, $(a-b)^{2N+1} < 0$ and $(a+b)^{2N+1} + (a-b)^{2N+1} < 0$. The first term in the expression of $\Phi(y)$ in (40) is a product of two strictly negative real numbers and is strictly positive. We also have $0 > a+b > a-b$, hence, again by oddness of $2N+1$, $(a+b)^{2N+1} > (a-b)^{2N+1}$ and the second term in (40) is a product of two strictly positive real numbers and is also strictly positive. Thus, $\Phi(y) > 0$ in the spectral gaps $(Y_{\min}^{4j+3}, Y_{\max}^{4j+2})$ and $(Y_{\min}^{4j+1}, Y_{\max}^{4j})$; it does not vanish in them.

From these two cases, we deduce that H_{2N+1} does not have any eigenvalue in the spectral gaps of H included in $[-V_0, 0]$. This proves the first point of Theorem 1.

Remark that in the second case the signs depend on the oddness of $2N+1$. There are slight changes to do in the even case and we present them in Appendix C.

3.3.2. *In the spectral bands.* Remark that from the expressions (48) and (51), similar arguments will give the number of zeroes of Φ in the even and odd spectral bands. Thus we will focus on the case of the even spectral bands and explain the differences with this case in the case of odd spectral bands all along the proof.

Using the expressions of $\Phi(y)$ given by (48) and (51), in order to count the zeroes of Φ in the spectral bands, we first have to study the properties of the function

$$\tilde{\varphi} : \begin{array}{ll} -c - \sigma(\mathbf{H}) & \rightarrow \mathbb{R} \\ y & \mapsto \text{Arg}(a+ib)(y+c). \end{array} \quad (52)$$

We prove the following result.

Proposition 1. *Let $p \geq 0$ and $c \geq c_p$. Then, for every $l \in \{0, \dots, p\}$,*

- (1) *if $l = 2j$ is even, the function $\tilde{\varphi}$ is a strictly decreasing homeomorphism from $[Y_{\max}^{2j}, Y_{\min}^{2j}]$ to $[0, \pi]$,*
- (2) *if $l = 2j+1$ is odd, the function $\tilde{\varphi}$ is a strictly increasing homeomorphism from $[Y_{\max}^{2j+1}, Y_{\min}^{2j+1}]$ to $[0, \pi]$.*

Before proving Proposition 1 we give the following lemma.

Lemma 1. *Let $p \geq 0$, $c \geq c_p$ and $h : [-c, 0] \rightarrow \mathbb{R}$ given by :*

$$\forall y \in [-c, 0], h(y) = -(\mathbf{U}\mathbf{U}')(\mathbf{y}+c) - y(\mathbf{V}\mathbf{V}')(\mathbf{y}+c) + (\mathbf{U}'\mathbf{V}')(\mathbf{y}+c) + (\mathbf{y}+c)(\mathbf{U}\mathbf{V})(\mathbf{y}+c). \quad (53)$$

Then, for every $l \in \{0, \dots, p\}$,

- (1) *if $l = 2j$ is even, for every $y \in [Y_{\max}^{2j}, Y_{\min}^{2j}]$, $h(y) > 0$,*
- (2) *if $l = 2j + 1$ is odd, for every $y \in [Y_{\max}^{2j+1}, Y_{\min}^{2j+1}]$, $h(y) < 0$.*

The proof of this lemma is quite technical and we postpone it until Appendix B.

Proof: (of Proposition 1).

Step 1. Let us start by computing the derivatives of the functions $y \mapsto \mathbf{U}(y+c)$, $y \mapsto \mathbf{U}'(y+c)$, $y \mapsto \mathbf{V}(y+c)$ and $y \mapsto \mathbf{V}'(y+c)$. For every $y \in \mathbb{R}$, $\mathbf{U}(y+c) = v'(y)u(y+c) - u'(y)v(y+c)$ and we have similar expressions for the three others functions. Hence, using also that u and v are solutions of the Airy equation :

$$\frac{d}{dy}\mathbf{U}(y+c) = -y\mathbf{V}(y+c) + \mathbf{U}'(y+c) \quad (54)$$

$$\frac{d}{dy}\mathbf{U}'(y+c) = -y\mathbf{V}'(y+c) + (y+c)\mathbf{U}(y+c) \quad (55)$$

$$\frac{d}{dy}\mathbf{V}(y+c) = -\mathbf{U}(y+c) + \mathbf{V}'(y+c) \quad (56)$$

$$\frac{d}{dy}\mathbf{V}'(y+c) = -\mathbf{U}'(y+c) + (y+c)\mathbf{V}(y+c) \quad (57)$$

where the $'$ denotes the derivation with respect to x in the expressions (13) and (14). Using (54), (55), (56) and (57), one gets :

$$\frac{d}{dy}(\mathbf{U}\mathbf{U}'\mathbf{V}\mathbf{V}')(\mathbf{y}+c) = (\mathbf{U}\mathbf{V}' + \mathbf{V}\mathbf{U}')(\mathbf{y}+c) \times h(\mathbf{y}). \quad (58)$$

Let $g : [-c, 0] \rightarrow \mathbb{R}$ given by

$$\forall y \in [-c, 0], g(y) = (\mathbf{U}\mathbf{V}' + \mathbf{V}\mathbf{U}')(\mathbf{y}+c). \quad (59)$$

Then, using again (54), (55), (56) and (57), we have

$$\forall y \in [-c, 0], \frac{d}{dy}g(y) = 2h(y) \quad (60)$$

and Lemma 1 gives the variations of g on each spectral band $[Y_{\max}^l, Y_{\min}^l]$. On each even spectral band ($l = 2j$), g is strictly increasing from $g(Y_{\max}^{2j}) = (\mathbf{V}\mathbf{U}')(\mathbf{Y}_{\max}^{2j}) < 0$ to $g(Y_{\min}^{2j}) = (\mathbf{U}\mathbf{V}')(\mathbf{Y}_{\min}^{2j}) > 0$, hence it vanishes at a unique point $Y_0^{2j} \in (Y_{\max}^{2j}, Y_{\min}^{2j})$. Similarly, on each odd spectral band, g is strictly decreasing and vanishes at a unique point $Y_0^{2j+1} \in (Y_{\max}^{2j+1}, Y_{\min}^{2j+1})$.

Step 2. We compute an explicit expression of the function $\tilde{\varphi}$ in terms of the functions \mathbf{U} , \mathbf{U}' , \mathbf{V} , \mathbf{V}' . We do not use the expression (16) but head back to the definition of φ . It turns out that the study of the variations of the expression we compute now is slightly simpler than the one of the expression (16).

Assume that $y \in [Y_{\max}^l, Y_{\min}^l]$ for some $l \in \{0, \dots, p\}$. Then,

$$\begin{aligned} |(a+ib)(y+c)| &= |(\mathbf{U}\mathbf{V}' + \mathbf{U}'\mathbf{V} + 2i\sqrt{-\mathbf{U}\mathbf{U}'\mathbf{V}\mathbf{V}'})(\mathbf{y}+c)| \\ &= (((\mathbf{U}\mathbf{V}' + \mathbf{U}'\mathbf{V})(\mathbf{y}+c))^2 - 4(\mathbf{U}\mathbf{U}'\mathbf{V}\mathbf{V}')(\mathbf{y}+c))^{\frac{1}{2}} \\ &= |(\mathbf{U}\mathbf{V}' - \mathbf{U}'\mathbf{V})(\mathbf{y}+c)| = 1 \end{aligned} \quad (61)$$

since the Wronskian of U and V is equal to 1. Moreover, since $2\sqrt{-UU'VV'}(y+c) \geq 0$, $\text{Arg}(a+ib)(y+c) \in [0, \pi]$. If $l = 2j$ is even, $g(y) < 0$ on $[Y_{\max}^{2j}, Y_0^{2j}]$ and

$$\forall y \in [Y_{\max}^{2j}, Y_0^{2j}], \quad \tilde{\varphi}(y) = \pi + \text{Arctan}\left(\frac{b}{a}\right)(y+c). \quad (62)$$

On $(Y_0^{2j}, Y_{\min}^{2j}]$, $g(y) > 0$ and

$$\forall y \in (Y_0^{2j}, Y_{\min}^{2j}], \quad \tilde{\varphi}(y) = \text{Arctan}\left(\frac{b}{a}\right)(y+c). \quad (63)$$

Since $(a+ib)(Y_0^{2j}+c) = ib(Y_0^{2j}+c)$, $\text{Arg}(a+ib)(Y_0^{2j}+c) = \frac{\pi}{2}$ and the function $\tilde{\varphi}$ is continuous on $[Y_{\max}^{2j}, Y_{\min}^{2j}]$.

If $l = 2j+1$ is odd, similarly,

$$\tilde{\varphi}(y) = \begin{cases} \text{Arctan}\left(\frac{b}{a}\right)(y+c) & \text{if } y \in [Y_{\max}^{2j+1}, Y_0^{2j+1}] \\ \pi + \text{Arctan}\left(\frac{b}{a}\right)(y+c) & \text{if } y \in (Y_0^{2j+1}, Y_{\min}^{2j+1}] \end{cases} \quad (64)$$

and again, since, $\text{Arg}(a+ib)(Y_0^{2j+1}+c) = \frac{\pi}{2}$, the function $\tilde{\varphi}$ is continuous on $[Y_{\max}^{2j+1}, Y_{\min}^{2j+1}]$.

Step 3. It remains to prove the monotonicity assertions to prove Proposition 1. For every $y \in [Y_{\max}^l, Y_{\min}^l]$, let

$$f(y) = \left(\frac{2\sqrt{-UU'VV'}}{UV' + U'V} \right) (y+c).$$

Note that $f = \tan(2\tilde{\varphi})$. Then, using (58) and (60),

$$\begin{aligned} \frac{d}{dy} f(y) &= \frac{2 \frac{d}{dy} (-UU'VV')(y+c)}{2\sqrt{-UU'VV'}} g(y) - 2\sqrt{-UU'VV'}(y+c) \frac{d}{dy} g(y) \\ &= \frac{h(y) (4(UU'VV')(y+c) - (g(y))^2)}{(g(y))^2 \sqrt{-UU'VV'}(y+c)} \\ &= \frac{h(y) (-(UV' - VU')(y+c))^2}{(g(y))^2 \sqrt{-UU'VV'}(y+c)} \\ &= \frac{-h(y)}{(g(y))^2 \sqrt{-UU'VV'}(y+c)}. \end{aligned}$$

since the Wronskian of U and V is equal to 1. Using Lemma 1, $\frac{d}{dy} f$ is strictly negative on each even spectral band and is strictly positive on each odd spectral band. Hence, f is strictly decreasing on each even spectral band and by (62) and (63), $\tilde{\varphi}$ is strictly decreasing from $[Y_{\max}^{2j}, Y_{\min}^{2j}]$ to $[\pi, 0]$. Since it is continuous, point (1) of Proposition 1 follows. Similarly, f is strictly increasing on each odd spectral band and by (64) and continuity proven at Step 2, point (2) of Proposition 1 follows. \square

Notation. We set, for every $m \in \{1, \dots, 2N\}$,

$$y_m^\pm = \tilde{\varphi}^{-1} \left(\frac{(2m \pm 1)\pi}{2(2N+1)} \right). \quad (65)$$

Proof: (of Theorem 1). We count the number of zeroes of Φ in an even spectral band $[Y_{\max}^{2j}, Y_{\min}^{2j}]$, $2j \in \{0, \dots, p\}$. The case of an odd spectral band is similar and we give the necessary changes to the proof of the even case at the end of this proof.

Step 1. By Proposition 1, $\tilde{\varphi}$ is a strictly decreasing homeomorphism from $[Y_{\max}^{2j}, Y_{\min}^{2j}]$ to $[0, \pi]$ with $\tilde{\varphi}(Y_{\max}^{2j}) = \pi$ and $\tilde{\varphi}(Y_{\min}^{2j}) = 0$. Hence, the function $y \mapsto \tan((2N+1)\tilde{\varphi}(y))$

- (1) vanishes at Y_{\max}^{2j} ;
- (2) is continuous, strictly decreasing on $[Y_{\max}^{2j}, y_{2N}^+)$ and tends to $-\infty$ when y tends to $(y_{2N}^+)^-$;
- (3) is continuous and strictly decreasing from $+\infty$ to $-\infty$ on each interval (y_m^+, y_m^-) for $m \in \{1, \dots, 2N\}$;
- (4) is continuous, strictly decreasing on $(y_1^-, Y_{\min}^{2j}]$ and tends to $+\infty$ when y tends to $(y_1^-)^+$;
- (5) vanishes at Y_{\min}^{2j} .

By the intermediate value theorem, the function $y \mapsto \tan((2N+1)\tilde{\varphi}(y))$ has exactly $2N+2$ zeroes in the interval $[Y_{\max}^{2j}, Y_{\min}^{2j}]$.

Step 2. The function k defined at (47) is strictly increasing from $-\infty$ to $+\infty$ on the interval $[Y_{\max}^{2j}, Y_{\min}^{2j}]$.

The function $x \mapsto \frac{x^2-1}{x^2+1}$ is continous on \mathbb{R} , even and it is strictly increasing from -1 to 1 on $[0, +\infty)$. Hence, $y \mapsto \frac{(k(y))^2-1}{(k(y))^2+1}$ is strictly positive on $[Y_{\max}^{2j}, k^{-1}(-1))$, strictly negative on $(k^{-1}(-1), k^{-1}(1))$, strictly positive on $(k^{-1}(1), Y_{\min}^{2j}]$ and vanishes only at the points $k^{-1}(-1)$ and $k^{-1}(1)$. It is also strictly decreasing from 1 to -1 on $[Y_{\max}^{2j}, k^{-1}(0)]$ and strictly increasing from -1 to 1 on $[k^{-1}(0), Y_{\min}^{2j}]$.

Let m_{\pm} the unique integer such that $k^{-1}(\pm 1) \in (y_{m_{\pm}}^+, y_{m_{\pm}}^-)$. Then, the function

$$y \mapsto \frac{(k(y))^2 - 1}{(k(y))^2 + 1} \tan((2N+1)\tilde{\varphi}(y))$$

- (1) vanishes at Y_{\max}^{2j} ;
- (2) is continuous, strictly decreasing on $[Y_{\max}^{2j}, y_{2N}^+)$ and tends to $-\infty$ when y tends to $(y_{2N}^+)^-$;
- (3) is continuous and strictly decreasing from $+\infty$ to $-\infty$ on each interval (y_m^+, y_m^-) for $m \in \{1, \dots, m_- - 1\}$;
- (4) is continuous on $(y_{m_-}^+, y_{m_-}^-)$, strictly decreasing from $+\infty$ to 0 on $(y_{m_-}^+, k^{-1}(-1)]$, negative on $[k^{-1}(-1), \tilde{\varphi}^{-1}(\frac{m-\pi}{2N+1})]$ and strictly increasing from 0 to $+\infty$ on $[\tilde{\varphi}^{-1}(\frac{m-\pi}{2N+1}), y_{m_-}^-)$, if $k^{-1}(-1) < \tilde{\varphi}^{-1}(\frac{m-\pi}{2N+1})$ (and the same variations if $k^{-1}(-1) > \tilde{\varphi}^{-1}(\frac{m-\pi}{2N+1})$, exchanging these two real numbers in the previous intervals bounds) ;
- (5) is continuous and strictly increasing from $-\infty$ to $+\infty$ on each interval (y_m^+, y_m^-) for $m \in \{m_- + 1, \dots, m_+ - 1\}$;
- (6) is continuous on $(y_{m_+}^+, y_{m_+}^-)$, strictly increasing from $-\infty$ to 0 on $(y_{m_+}^+, k^{-1}(1)]$, positive on $[k^{-1}(1), \tilde{\varphi}^{-1}(\frac{m+\pi}{2N+1})]$ and strictly decreasing from 0 to $-\infty$ on $[\tilde{\varphi}^{-1}(\frac{m+\pi}{2N+1}), y_{m_+}^-)$, if $k^{-1}(1) < \tilde{\varphi}^{-1}(\frac{m+\pi}{2N+1})$ (and the same variations if $k^{-1}(1) > \tilde{\varphi}^{-1}(\frac{m+\pi}{2N+1})$, exchanging these two real numbers in the previous intervals bounds) ;
- (7) is continuous and strictly decreasing from $+\infty$ to $-\infty$ on each interval (y_m^+, y_m^-) for $m \in \{m_+ + 1, \dots, 2N\}$;

(8) is continuous, strictly decreasing on $(y_1^-, Y_{\min}^{2j}]$ and tends to $+\infty$ when y tends to $(y_1^-)^+$;

(9) vanishes at Y_{\min}^{2j} .

Since $k^{-1}(-1) \neq \tilde{\varphi}^{-1}\left(\frac{m-\pi}{2N+1}\right)$ and $k^{-1}(1) \neq \tilde{\varphi}^{-1}\left(\frac{m+\pi}{2N+1}\right)$, the function

$$y \mapsto \frac{(k(y))^2 - 1}{(k(y))^2 + 1} \tan((2N+1)\tilde{\varphi}(y))$$

has exactly 2 zeroes in both intervals (y_{m-}^+, y_{m-}^-) and (y_{m+}^+, y_{m+}^-) . Hence, the function $y \mapsto \frac{(k(y))^2 - 1}{(k(y))^2 + 1} \tan((2N+1)\tilde{\varphi}(y))$ has exactly $2N+4$ zeroes in the interval $[Y_{\max}^{2j}, Y_{\min}^{2j}]$. The rest of the proof does not change if $k^{-1}(-1) \in [Y_{\max}^{2j}, y_{2N}^+)$ or $k^{-1}(1) \in (y_1^-, Y_{\min}^{2j}]$.

Step 3. We remark that

$$\frac{2k(k^{-1}(\pm 1))}{1 + (k(k^{-1}(\pm 1)))^2} = \pm 1$$

and

$$\lim_{y \rightarrow (Y_{\max}^{2j})^+} \frac{2k(y)}{1 + (k(y))^2} = \lim_{y \rightarrow (Y_{\min}^{2j})^-} \frac{2k(y)}{1 + (k(y))^2} = 0.$$

Moreover, the function $y \mapsto \frac{2k(y)}{1 + (k(y))^2}$ is strictly decreasing on $[Y_{\max}^{2j}, k^{-1}(-1)]$, strictly increasing on $[k^{-1}(-1), k^{-1}(1)]$ and strictly decreasing on $[k^{-1}(1), Y_{\min}^{2j}]$. Hence, considering the monotonicity and the limits $\pm\infty$ of the function

$$y \mapsto \frac{(k(y))^2 - 1}{(k(y))^2 + 1} \tan((2N+1)\tilde{\varphi}(y))$$

on each of the sub intervals $[Y_{\max}^{2j}, Y_{\min}^{2j}]$ defined at Step 2, the function

$$y \mapsto \frac{2k(y)}{1 + (k(y))^2} + \frac{(k(y))^2 - 1}{(k(y))^2 + 1} \tan((2N+1)\tilde{\varphi}(y))$$

has the same number of zeroes as the function

$$y \mapsto \frac{(k(y))^2 - 1}{(k(y))^2 + 1} \tan((2N+1)\tilde{\varphi}(y))$$

on each of these sub intervals. Hence, the function

$$y \mapsto \frac{2k(y)}{1 + (k(y))^2} + \frac{(k(y))^2 - 1}{(k(y))^2 + 1} \tan((2N+1)\tilde{\varphi}(y))$$

has exactly $2N+4$ zeroes in the interval $[Y_{\max}^{2j}, Y_{\min}^{2j}]$.

Step 4. The function $y \mapsto \frac{1}{2^{2N+1}}((a+ib)^{2N+1} + (a-ib)^{2N+1})(y+c) = 2 \cos((2N+1)\tilde{\varphi}(y+c))$ is continuous and vanishes on $[Y_{\max}^{2j}, Y_{\min}^{2j}]$ only at the points y_m^+ , $m \in \{0, \dots, 2N\}$. It does not vanish and is of constant sign on each interval (y_m^+, y_m^-) for $m \in \{1, \dots, 2N\}$. Moreover $b(Y_{\max}^{2j} + c) = b(Y_{\min}^{2j} + c) = 0$, $a(Y_{\max}^{2j} + c) < 0$ and $a(Y_{\min}^{2j} + c) > 0$.

The function $y \mapsto (\alpha + \beta)(y+c)$ is strictly positive on the interval $(Y_{\max}^{2j}, Y_{\min}^{2j})$. Moreover, $\beta(Y_{\max}^{2j} + c) = \beta(Y_{\min}^{2j} + c) = 0$ and

$$\lim_{y \rightarrow (Y_{\max}^{2j})^+} \alpha(y+c) = \lim_{y \rightarrow (Y_{\min}^{2j})^-} \alpha(y+c) = +\infty.$$

Hence, one already has that Φ has exactly $2N+2$ zeroes on the interval (y_{2N}^+, y_1^-) .

Since $y \mapsto \tan((2N+1)\tilde{\varphi}(y))$ is strictly negative on $(Y_{\max}^{2j}, y_{2N}^+)$ and vanishes at Y_{\max}^{2j} , one deduces from all what precedes that either $\Phi(Y_{\max}^{2j}) > 0$ or $\Phi(y)$ tends to $+\infty$ when y tends to $(Y_{\max}^{2j})^+$. Since by definition of Φ it is a continuous function on $[-c, 0]$, only the first case occurs. Hence, since $y \mapsto \cos((2N+1)\tilde{\varphi}(y))$ is strictly negative on $(Y_{\max}^{2j}, y_{2N}^+)$, Φ is strictly positive on this interval and does not vanish on it.

Since $y \mapsto \tan((2N+1)\tilde{\varphi}(y))$ is strictly positive on (y_1^-, Y_{\min}^{2j}) and vanishes at Y_{\min}^{2j} , one deduces that either $\Phi(Y_{\min}^{2j}) > 0$ or $\Phi(y)$ tends to $+\infty$ when y tends to $(Y_{\min}^{2j})^-$. Since Φ is continuous, only the first case occurs. In particular, since $y \mapsto \cos((2N+1)\tilde{\varphi}(y))$ is strictly positive on the interval (y_1^-, Y_{\min}^{2j}) , Φ is strictly positive on this interval and thus does not vanish on it.

One concludes that Φ has exactly $2N+2$ zeroes in the interval $[Y_{\max}^{2j}, Y_{\min}^{2j}]$, which proves Theorem 1 in the case of an even spectral band.

For an odd spectral band, $\tilde{\varphi}$ is a strictly increasing homeomorphism from $[Y_{\max}^{2j+1}, Y_{\min}^{2j+1}]$ to $[0, \pi]$. Hence, Step 1 is the same as in the even case, replacing “decreasing” by “increasing”, changing $-\infty$ into $+\infty$ and vice versa and taking care of the order of the numbers $y_m^\pm = \tilde{\varphi}^{-1}\left(\frac{(2m\pm 1)\pi}{2(2N+1)}\right)$ which is reversed.

The function \tilde{k} is a strictly decreasing function from $+\infty$ to $-\infty$ on $[Y_{\max}^{2j+1}, Y_{\min}^{2j+1}]$, hence Step 2 and Step 3 will not change except that the order of the numbers $\tilde{k}^{-1}(-1)$ and $\tilde{k}^{-1}(1)$ has to be changed.

Finally, Step 4 is similar, again inverting the ordering of the subintervals since $\tilde{\varphi}$ is now increasing. It finishes the proof of Theorem 1. \square

4. PROOF OF THEOREM 2

The main ingredient used to count the eigenvalues of \mathbf{H}_{2N+1} under a fixed real number is that we know from Section 3.3 that these eigenvalues are in the spectral bands of \mathbf{H} , situated between two singularities of the function $\mathbf{E} \mapsto \tan((2N+1)\varphi(\mathbf{E}))$.

We also need more notations for the proof of Theorem 2. These notations will also be used in the proof of Lemma 1. Let Ai and Bi denote the usual Airy functions.

Notation. We denote by $\{-a_j\}_{j \geq 1}$ the set of the zeroes of Ai and by $\{-\tilde{a}_j\}_{j \geq 1}$ the set of the zeroes of Ai' where the real numbers $-a_j$ and $-\tilde{a}_j$ are arranged in decreasing order. These sets are both subsets of $(-\infty, 0]$.

Let $j \geq 0$ and define the real numbers $\mathbf{a}_{2j} = \tilde{a}_{j+1}$ and $\mathbf{a}_{2j+1} = a_{j+1}$.

Proof: (of Theorem 2). We use the notations introduced in the proof of Theorem 1. Let $\mathbf{E} \in [-c, 0]$.

We start by counting the number of spectral bands of \mathbf{H} included in the interval $[-c, \mathbf{E}]$ and thus prove (18). Let $p \geq 0$. Using the results of [2, Proposition 6.1], the p -th spectral band of \mathbf{H} is centered at $-c + \mathbf{a}_p$. Hence, the number $p(\mathbf{E})$ of spectral bands of \mathbf{H} included in $[-c, \mathbf{E}]$ (of length $c + \mathbf{E}$) is the unique integer such that

$$\mathbf{a}_{p(\mathbf{E})} \leq c + \mathbf{E} \leq \mathbf{a}_{p(\mathbf{E})+1}. \quad (66)$$

With a similar argument as in the proof of [2, Proposition 3.1], we get, for every $j \geq 0$,

$$\frac{2}{3}(\tilde{a}_{j+1})^{\frac{3}{2}} \in \left[\frac{\pi}{4} + j\pi - \frac{7}{36(\frac{\pi}{6} + j\pi)}, \frac{\pi}{4} + j\pi + \frac{7}{36(\frac{\pi}{6} + j\pi)} \right]$$

and

$$\frac{2}{3}(a_{j+1})^{\frac{3}{2}} \in \left[\frac{3\pi}{4} + j\pi - \frac{5}{36(\frac{\pi}{6} + j\pi)}, \frac{3\pi}{4} + j\pi + \frac{5}{36(\frac{\pi}{6} + j\pi)} \right].$$

Combined with (66), it gives (18).

We set, for every $m \in \{1, \dots, 2N\}$,

$$e_m^\pm = \varphi^{-1} \left(\frac{(2m \pm 1)\pi}{2(2N+1)} \right). \quad (67)$$

In an even spectral band. Let $j \geq 0$. Let $\mathbf{E} \in [\mathbf{E}_{\min}^{2j}, \mathbf{E}_{\max}^{2j}]$. From Proposition 1, φ defined at (15) having the opposite variations on $[\mathbf{E}_{\min}^p, \mathbf{E}_{\max}^p]$ to $\tilde{\varphi}$ on $[Y_{\max}^p, Y_{\min}^p]$, it is strictly increasing on $[\mathbf{E}_{\min}^{2j}, \mathbf{E}_{\max}^{2j}]$.

Let $m_{\mathbf{E}} \in \{1, \dots, 2N\}$ be the unique integer such that $\mathbf{E} \in [e_{m_{\mathbf{E}}}^-, e_{m_{\mathbf{E}}}^+]$ and let $m_{\mathbf{E}} = 0$ if $\mathbf{E} \in [\mathbf{E}_{\min}^{2j}, e_1^-]$ and $m_{\mathbf{E}} = 2N$ if $\mathbf{E} \in (e_{2N}^+, \mathbf{E}_{\max}^{2j}]$.

From the proof of Theorem 1, we already know that in each interval (e_m^-, e_m^+) for $m \in \{1, \dots, 2N\}$, there is exactly one eigenvalue of \mathbf{H} , except for $m = m_{\pm}$ for which there are 2 eigenvalues of \mathbf{H} . We also know that there is no eigenvalues of \mathbf{H} in $[\mathbf{E}_{\min}^{2j}, e_1^-]$ and in $(e_{2N}^+, \mathbf{E}_{\max}^{2j}]$ which explains the definition of $m_{\mathbf{E}}$. Hence, there are exactly $m_{\mathbf{E}} + n_{\mathbf{E}}$ eigenvalues of \mathbf{H} in the interval $[\mathbf{E}_{\min}^{2j}, \mathbf{E}]$ with $n_{\mathbf{E}} \in \{0, 1, 2\}$.

But, since φ is strictly increasing,

$$\frac{(2m_{\mathbf{E}} - 1)\pi}{2(2N+1)} \leq \varphi(\mathbf{E}) \leq \frac{(2m_{\mathbf{E}} + 1)\pi}{2(2N+1)}$$

and

$$\frac{2N+1}{\pi} \varphi(\mathbf{E}) - \frac{1}{2} \leq m_{\mathbf{E}} \leq \frac{2N+1}{\pi} \varphi(\mathbf{E}) + \frac{1}{2}. \quad (68)$$

Hence,

$$\lim_{N \rightarrow +\infty} \frac{1}{2(2N+1)} (m_{\mathbf{E}} + n_{\mathbf{E}}) = \frac{1}{2\pi} \varphi(\mathbf{E}). \quad (69)$$

In an odd spectral band. The argument is similar to the even case, except that φ is strictly decreasing as a consequence of Proposition 1. Let $j \geq 0$ and let $\mathbf{E} \in [\mathbf{E}_{\min}^{2j+1}, \mathbf{E}_{\max}^{2j+1}]$. We define $m_{\mathbf{E}}$ as in the even case except that we exchange the bounds of each subinterval of $[\mathbf{E}_{\min}^{2j+1}, \mathbf{E}_{\max}^{2j+1}]$ and we set $m_{\mathbf{E}} = 2N$ if $\mathbf{E} \in [\mathbf{E}_{\min}^{2j+1}, e_{2N}^+]$ and $m_{\mathbf{E}} = 0$ if $\mathbf{E} \in [e_1^-, \mathbf{E}_{\max}^{2j+1}]$.

Since φ is decreasing, as in the even case, the number of eigenvalues of \mathbf{H} in $[\mathbf{E}, \mathbf{E}_{\max}^{2j+1}]$ is equal to $m_{\mathbf{E}} + n_{\mathbf{E}}$ with $n_{\mathbf{E}} \in \{0, 1, 2\}$. Hence, using the result of Theorem 1, there are exactly $2N + 2 - (m_{\mathbf{E}} + n_{\mathbf{E}})$ eigenvalues of \mathbf{H} in the interval $[\mathbf{E}_{\min}^{2j+1}, \mathbf{E}]$.

We still have an inequality similar to (68) except that we exchange the upper and lower bounds, thus

$$\lim_{N \rightarrow +\infty} \frac{1}{2(2N+1)} (2N + 2 - (m_{\mathbf{E}} + n_{\mathbf{E}})) = \frac{1}{2} - \frac{1}{2\pi} \varphi(\mathbf{E}). \quad (70)$$

Conclusion. Since φ is a homeomorphism from each spectral band to $[0, \pi]$, from (70) and (69), we get that if \mathbf{E} is in a spectral gap of \mathbf{H} , the integrated density of states of \mathbf{H} , $\mathbf{I}(\mathbf{E})$, is equal to $\frac{1}{2}p(\mathbf{E})$, where $p(\mathbf{E})$ is the number of spectral bands included in $[-c, \mathbf{E}]$. Theorem 2 follows as this remark, (70) and (69) implies (17) and (18) has already been proven. \square

APPENDIX A. APPROXIMATIONS OF φ IN THE SPECTRAL BANDS

We start by proving (16). From (61) the complex number $(U'V + UV' + 2i\sqrt{-UU'VV'})(-\mathbf{E})$ is always of modulus 1 for $\mathbf{E} \in [-c, 0] \cap \sigma(\mathbf{H})$. Moreover, on the interior of each spectral band of \mathbf{H} , $U'V < 0$ and $UV' > 0$. Hence,

$$U'V + UV' + 2i\sqrt{-UU'VV'} = (\sqrt{-U'V} + i\sqrt{V'U})^2$$

and for every $\mathbf{E} \in [-c, 0] \cap \sigma(\mathbf{H})$,

$$\text{Arg}((U'V + UV' + 2i\sqrt{-UU'VV'})(-\mathbf{E})) = 2\text{Arg}((\sqrt{-U'V} + i\sqrt{V'U})(-\mathbf{E}))$$

and by positivity of $\sqrt{-U'V}$, (16) follows.

Now, we precise what we meant by “a squareroot behavior” in the introduction. We have the following result.

Proposition 2. *For every $c \geq c_p$ and every $i \in \{0, \dots, p\}$, there exist real numbers K_{\min}^i , K_{\max}^i and $\varepsilon > 0$ such that*

$$\forall \mathbf{E} \in \sigma(\mathbf{H}) \cap [\mathbf{E}_{\min}^i, \mathbf{E}_{\min}^i + \varepsilon], \quad \varphi(\mathbf{E}) = K_{\min}^i (\mathbf{E} - \mathbf{E}_{\min}^i)^{\frac{1}{2}} + o\left((\mathbf{E} - \mathbf{E}_{\min}^i)^{\frac{1}{2}}\right) \quad (71)$$

and

$$\forall \mathbf{E} \in \sigma(\mathbf{H}) \cap [\mathbf{E}_{\max}^i - \varepsilon, \mathbf{E}_{\max}^i], \quad \varphi(\mathbf{E}) = K_{\max}^i (\mathbf{E}_{\max}^i - \mathbf{E})^{\frac{1}{2}} + o\left((\mathbf{E}_{\max}^i - \mathbf{E})^{\frac{1}{2}}\right) \quad (72)$$

Proof: We prove the result for \mathbf{E}_{\min}^i and $i = 2l$ even. The other cases lead to similar computations. In this case, one has $U'(-\mathbf{E}_{\min}^{2l}) = 0$ and since U is C^∞ one writes for \mathbf{E} in a neighborhood $[\mathbf{E}_{\min}^{2l}, \mathbf{E}_{\min}^{2l} + \varepsilon]$ of \mathbf{E}_{\min}^{2l} ,

$$\begin{aligned} U'(-\mathbf{E}) &= U'(-\mathbf{E}_{\min}^{2l}) + U''(-\mathbf{E}_{\min}^{2l}) \cdot (-\mathbf{E} + \mathbf{E}_{\min}^{2l}) + o(\mathbf{E} - \mathbf{E}_{\min}^{2l}) \\ &= U''(-\mathbf{E}_{\min}^{2l}) \cdot (-\mathbf{E} + \mathbf{E}_{\min}^{2l}) + o(\mathbf{E} - \mathbf{E}_{\min}^{2l}), \end{aligned}$$

hence, since U satisfies the Airy equation and $V(-\mathbf{E}_{\min}^{2l}) \neq 0$,

$$\begin{aligned} (-U'V)(-\mathbf{E}) &= (U''V)(-\mathbf{E}_{\min}^{2l}) \cdot (\mathbf{E} - \mathbf{E}_{\min}^{2l}) + o(\mathbf{E} - \mathbf{E}_{\min}^{2l}) \\ &= (-\mathbf{E}_{\min}^{2l})(UV)(-\mathbf{E}_{\min}^{2l}) \cdot (\mathbf{E} - \mathbf{E}_{\min}^{2l}) + o(\mathbf{E} - \mathbf{E}_{\min}^{2l}). \end{aligned}$$

Then, using (16), the usual power series of Arctan and $x \mapsto \sqrt{1+x}$ near 0 and the fact that $(V'U)(-\mathbf{E}_{\min}^{2l}) \neq 0$, we get

$$\varphi(\mathbf{E}) = \left(-\mathbf{E}_{\min}^{2l} \frac{(UV)(-\mathbf{E}_{\min}^{2l})}{(V'U)(-\mathbf{E}_{\min}^{2l})}\right)^{\frac{1}{2}} (\mathbf{E} - \mathbf{E}_{\min}^{2l})^{\frac{1}{2}} + o\left((\mathbf{E} - \mathbf{E}_{\min}^{2l})^{\frac{1}{2}}\right),$$

hence (71) with

$$K_{\min}^{2l} = \left(-\mathbf{E}_{\min}^{2l} \frac{V(-\mathbf{E}_{\min}^{2l})}{V'(-\mathbf{E}_{\min}^{2l})}\right)^{\frac{1}{2}}.$$

□

Note that the constants K_{\star}^i , $\star \in \{\min, \max\}$ depend on c and i and they are of order $(-\mathbf{E}_{\star}^i)^{\frac{1}{2}}$ hence larger for the spectral band edges far from 0 (which corresponds to the first bands) than for the spectral band edges close to 0. It explains, for example, the steepness of the IDS near the spectral band edges of the first spectral band compared to the second one in Figure 2.

We finish this first appendix by giving the heuristic of an approximate formula for φ and its derivative φ' which is the Density Of States. This formula is a good approximation of the IDS in the interior of the first spectral bands, for c large and \mathbf{E} far from 0. Let \mathbf{E} in $[-c, 0]$.

First, we replace $U(x)$ by $\frac{1}{\pi}(Bi'(-c - \mathbf{E})Ai(x) - Ai'(-c - \mathbf{E})Bi(x))$ and we replace $V(x)$ by $\frac{1}{\pi}(Ai(-c - \mathbf{E})Bi(x) - Bi(-c - \mathbf{E})Ai(x))$.

Next, we use the expressions of u , u' , v and v' in term of the Airy functions and the P and Q functions given in [2, Section 3.1]. A rough, but sufficient approximate value for these functions on the negative real half-line is obtained for $P = 1$ and $Q = 0$. It leads to replace $Ai(-c - \mathbf{E})$ by $\pi^{-\frac{1}{2}}(c + \mathbf{E})^{-\frac{1}{4}} \sin(\zeta + \frac{\pi}{4})$, $Ai'(-c - \mathbf{E})$ by $-\pi^{-\frac{1}{2}}(c + \mathbf{E})^{\frac{1}{4}} \cos(\zeta + \frac{\pi}{4})$, $Bi(-c - \mathbf{E})$ by $\pi^{-\frac{1}{2}}(c + \mathbf{E})^{-\frac{1}{4}} \cos(\zeta + \frac{\pi}{4})$ and $Bi'(-c - \mathbf{E})$ by $-\pi^{-\frac{1}{2}}(c + \mathbf{E})^{\frac{1}{4}} \sin(\zeta + \frac{\pi}{4})$ with $\zeta = \frac{2}{3}(c + E)^{\frac{3}{2}}$. These approximates are not precise for \mathbf{E} close to 0 but as soon as we move away from 0 they become better.

On the positive real half-line, we replace $Ai(-\mathbf{E})$ by $\pi^{\frac{1}{2}}(-\mathbf{E})^{-\frac{1}{4}} e^{-\frac{2}{3}(-\mathbf{E})^{\frac{3}{2}}}$, $Ai'(-\mathbf{E})$ by $-\pi^{\frac{1}{2}}(-\mathbf{E})^{\frac{1}{4}} e^{-\frac{2}{3}(-\mathbf{E})^{\frac{3}{2}}}$, $Bi(-\mathbf{E})$ by $\pi^{\frac{1}{2}}(-\mathbf{E})^{-\frac{1}{4}} e^{\frac{2}{3}(-\mathbf{E})^{\frac{3}{2}}}$ and $Bi'(-\mathbf{E})$ by $\pi^{\frac{1}{2}}(-\mathbf{E})^{\frac{1}{4}} e^{\frac{2}{3}(-\mathbf{E})^{\frac{3}{2}}}$.

Hence, one gets for $\frac{U'V}{UV'}$ the following approximation

$$\frac{U'V}{UV'}(-\mathbf{E}) \sim \frac{\sin(\zeta + \frac{\pi}{4}) \cos(\zeta + \frac{\pi}{4}) e^{\frac{4}{3}(-\mathbf{E})^{\frac{3}{2}}} - 2 + \sin(\zeta + \frac{\pi}{4}) \cos(\zeta + \frac{\pi}{4}) e^{-\frac{4}{3}(-\mathbf{E})^{\frac{3}{2}}}}{\sin(\zeta + \frac{\pi}{4}) \cos(\zeta + \frac{\pi}{4}) e^{\frac{4}{3}(-\mathbf{E})^{\frac{3}{2}}} + 2 + \sin(\zeta + \frac{\pi}{4}) \cos(\zeta + \frac{\pi}{4}) e^{-\frac{4}{3}(-\mathbf{E})^{\frac{3}{2}}}},$$

which simplifies into

$$\frac{U'V}{UV'}(-\mathbf{E}) \sim \frac{\sin(2\zeta + \frac{\pi}{2}) - \frac{1}{\cosh \frac{4}{3}(-\mathbf{E})^{\frac{3}{2}}}}{\sin(2\zeta + \frac{\pi}{2}) + \frac{1}{\cosh \frac{4}{3}(-\mathbf{E})^{\frac{3}{2}}}}.$$

Moreover, if we assume that

$$\left| \sin \frac{4}{3}(c + \mathbf{E})^{\frac{3}{2}} \right| \leq \frac{1}{\cosh \frac{4}{3}(-\mathbf{E})^{\frac{3}{2}}}$$

then, using (16), we get that

$$\tan \varphi(\mathbf{E}) \sim \sqrt{\frac{\frac{1}{\cosh \frac{4}{3}(-\mathbf{E})^{\frac{3}{2}}} - \sin(2\zeta + \frac{\pi}{2})}{\sin(2\zeta + \frac{\pi}{2}) + \frac{1}{\cosh \frac{4}{3}(-\mathbf{E})^{\frac{3}{2}}}}}.$$

Finally we get the approximation

$$\varphi(\mathbf{E}) \sim \text{Arctan} \left(\left(\frac{1 - \cos(\frac{4}{3}(c + \mathbf{E})^{\frac{3}{2}}) \cosh \frac{4}{3}(-\mathbf{E})^{\frac{3}{2}}}{1 + \cos(\frac{4}{3}(c + \mathbf{E})^{\frac{3}{2}}) \cosh \frac{4}{3}(-\mathbf{E})^{\frac{3}{2}}} \right)^{\frac{1}{2}} \right). \quad (73)$$

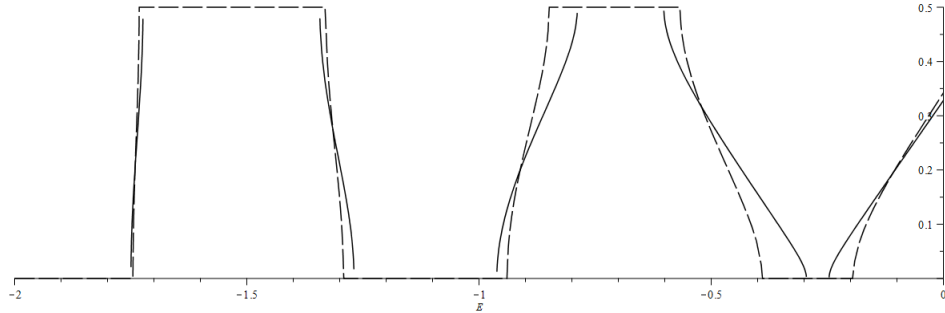


FIGURE 3. The function φ and its approximation given in (73) on $[-2, 0]$ for $c = 15$. The solid line represents the approximation divided by π and the dashed line represents φ divided by 2π .

As expected, the Figure 3 illustrates that the approximation given in (73) is better for the spectral bands far from 0 than for the bands close to 0.

Moreover, if we derive the approximation (73) with respect to \mathbf{E} we find an approximation for the Density Of States $\varphi'(\mathbf{E})$ which, as recalled in the introduction, is usually the interesting quantity in the physics literature.

$$\varphi'(\mathbf{E}) \sim \frac{1}{1 + \cosh \frac{4}{3}(-\mathbf{E})^{\frac{3}{2}} \cos \frac{4}{3}(\mathbf{c} + \mathbf{E})^{\frac{3}{2}}}. \quad (74)$$

APPENDIX B. PROOF OF LEMMA 1

To prove Lemma 1, we use well-known properties of the classical Airy functions Ai and Bi and their approximations combined with results from [2]. The idea is the following : the p -th spectral band of \mathbf{H} is centered at $-\mathbf{c} + \mathbf{a}_p$, hence we prove that the value of $h(-\mathbf{a}_p)$ is strictly positive when p is even and strictly negative when p is odd. Since the length of each spectral band is exponentially small, it implies, using Taylor formula, that the sign of h does not change on each spectral band. We focus on the case p even, the odd case is completely similar.

To start, note that one has the expression of u and v in terms of Ai and Bi :

$$\forall x \in \mathbb{R}, u(x) = \pi(Bi'(0)Ai(x) - Ai'(0)Bi(x))$$

and

$$\forall x \in \mathbb{R}, v(x) = \pi(Ai(0)Bi(x) - Bi(0)Ai(x)).$$

Also recall that the Wronskian of Ai and Bi is equal to $\frac{1}{\pi}$. Let $j \geq 0$, and $\mathbf{c} \geq c_{2j}$. Since $Ai'(-\tilde{a}_{j+1}) = 0$,

$$U(-\tilde{a}_{j+1} + \mathbf{c}) = \pi Bi'(-\tilde{a}_{j+1})Ai(-\tilde{a}_{j+1} + \mathbf{c}); \quad (75)$$

$$U'(-\tilde{a}_{j+1} + \mathbf{c}) = \pi Bi'(-\tilde{a}_{j+1})Ai'(-\tilde{a}_{j+1} + \mathbf{c}); \quad (76)$$

$$V(-\tilde{a}_{j+1} + \mathbf{c}) = \pi(Ai(-\tilde{a}_{j+1})Bi(-\tilde{a}_{j+1}) - Bi(-\tilde{a}_{j+1})Ai(-\tilde{a}_{j+1} + \mathbf{c})); \quad (77)$$

$$V'(-\tilde{a}_{j+1} + \mathbf{c}) = \pi(Ai(-\tilde{a}_{j+1})Bi'(-\tilde{a}_{j+1}) - Bi(-\tilde{a}_{j+1})Ai'(-\tilde{a}_{j+1} + \mathbf{c})). \quad (78)$$

Hence,

$$h(-\tilde{a}_{j+1}) = \pi^2 [(\tilde{a}_{j+1}(Bi(-\tilde{a}_{j+1}))^2 - (Bi'(-\tilde{a}_{j+1}))^2)(AiAi')(-\tilde{a}_{j+1} + \mathbf{c}) \quad (79)$$

$$+ \tilde{a}_{j+1}(Ai(-\tilde{a}_{j+1}))^2(BiBi')(-\tilde{a}_{j+1} + \mathbf{c}) \quad (80)$$

$$- \frac{1}{\pi}(AiBi)(-\tilde{a}_{j+1}) \quad (81)$$

$$+ (AiBi')(-\tilde{a}_{j+1})(Ai'Bi')(-\tilde{a}_{j+1} + \mathbf{c}) \quad (82)$$

$$- (BiBi')(-\tilde{a}_{j+1})(Ai'(-\tilde{a}_{j+1} + \mathbf{c}))^2 \quad (83)$$

$$+ (-\tilde{a}_{j+1} + \mathbf{c})(AiBi')(-\tilde{a}_{j+1})(AiBi)(-\tilde{a}_{j+1} + \mathbf{c}) \quad (84)$$

$$- (-\tilde{a}_{j+1} + \mathbf{c})(BiBi')(-\tilde{a}_{j+1})(Ai(-\tilde{a}_{j+1} + \mathbf{c}))^2]. \quad (85)$$

One already sees that in the expression of $h(-\tilde{a}_{j+1})$, the dominant term when \mathbf{c} is large is (80), hence positive. But our result is stated not for \mathbf{c} arbitrarily large, but for every $\mathbf{c} \geq c_{2j}$. Since it is increasing in \mathbf{c} , we may assume in the sequel that $\mathbf{c} = c_{2j}$ and the result follows for any $\mathbf{c} \geq c_{2j}$.

First, for $j = 0$, one has $-\tilde{a}_1 \simeq -1.088$, $c_0 \simeq 1.515$ and $h(-\tilde{a}_1) \simeq 1.428 > 0$. In the sequel, we assume $j \geq 1$.

Using [1, 10.4.95],

$$\left| -\tilde{a}_{j+1} - \left(- \left(\frac{3\pi}{8} (4j+3) \right)^{\frac{2}{3}} \right) \right| \leq \frac{5}{48} \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{4}{3}}. \quad (86)$$

Using [1, 10.4.97],

$$\left| Ai(-\tilde{a}_{j+1}) - \frac{(-1)^j}{\sqrt{\pi}} \left(\frac{3\pi}{8} (4j+3) \right)^{\frac{1}{6}} \right| \leq \frac{5}{48} \frac{1}{\sqrt{\pi}} \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{11}{6}}. \quad (87)$$

By [1, 10.4.64] and (86),

$$\left| Bi(-\tilde{a}_{j+1}) - \frac{(-1)^{j+1}}{\sqrt{\pi}} \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{1}{6}} \right| \leq \frac{385}{4608} \frac{1}{\sqrt{\pi}} \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{13}{6}}. \quad (88)$$

Using [1, 10.4.67],

$$\left| Bi'(-\tilde{a}_{j+1}) - \frac{3}{2} \frac{(-1)^j}{\sqrt{\pi}} \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{5}{4}} \right| \leq \frac{7315}{663552} \frac{1}{\sqrt{\pi}} \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{17}{6}}. \quad (89)$$

Combining (86) and [2, Proposition 3.1], one also has

$$\begin{aligned} \left| (-\tilde{a}_{j+1} + c_{2j}) - \frac{2}{9} \left(\frac{3\pi}{2} \right)^{\frac{2}{3}} j^{-\frac{1}{3}} \right| &\leq \frac{5}{48} \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{4}{3}} + \left(\frac{7}{8\pi(j+\frac{1}{3})} \right)^{\frac{2}{3}} \\ &\leq 2 \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{2}{3}}. \end{aligned} \quad (90)$$

Note that

$$2 \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{2}{3}} \leq \frac{2}{9} \left(\frac{3\pi}{2} \right)^{\frac{2}{3}} j^{-\frac{1}{3}} + 2 \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{2}{3}} \leq \frac{4}{9} \left(\frac{3\pi}{2} \right)^{\frac{2}{3}} j^{-\frac{1}{3}}.$$

Hence

$$\frac{1}{\pi} \frac{8}{27} j^{\frac{1}{2}} \leq \frac{3}{2} \left(\frac{2}{9} \left(\frac{3\pi}{2} \right)^{\frac{2}{3}} j^{-\frac{1}{3}} + 2 \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{2}{3}} \right)^{-\frac{3}{2}} \leq \frac{9\pi}{32\sqrt{2}} (4j+3), \quad (91)$$

$$\frac{1}{2\sqrt{2}} (4j+3)^{-1} \leq \frac{4}{3} \left(\frac{2}{9} \left(\frac{3\pi}{2} \right)^{\frac{2}{3}} j^{-\frac{1}{3}} + 2 \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{2}{3}} \right)^{\frac{3}{2}} \leq \frac{16}{27} \pi j^{-\frac{1}{2}}, \quad (92)$$

$$\left(\frac{2}{9} \left(\frac{3\pi}{2} \right)^{\frac{2}{3}} j^{-\frac{1}{3}} + 2 \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{2}{3}} \right)^{\frac{1}{2}} \leq \frac{2}{3} \left(\frac{3\pi}{2} \right)^{\frac{1}{3}} j^{-\frac{1}{6}} \quad (93)$$

and

$$\left(\frac{2}{9} \left(\frac{3\pi}{2} \right)^{\frac{2}{3}} j^{-\frac{1}{3}} + 2 \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{2}{3}} \right)^{-\frac{1}{2}} \leq \frac{1}{\sqrt{2}} \left(\frac{3\pi}{8} (4j+3) \right)^{\frac{1}{3}}. \quad (94)$$

Using [1, 10.4.59 and 10.4.61], (91) and (92),

$$\left| (AiAi')(-\tilde{a}_{j+1} + c_{2j}) - \left(-\frac{1}{4\pi} e^{-2\pi(\frac{2}{9})^{\frac{3}{2}} j^{-\frac{1}{2}}} \right) \right| \leq \frac{5}{1024\sqrt{2}} (4j+3) e^{-\frac{1}{2\sqrt{2}(4j+3)}}. \quad (95)$$

Using [1, 10.4.63 and 10.4.66], (91) and (92),

$$\left| (BiBi')(-\tilde{a}_{j+1} + c_{2j}) - \frac{1}{\pi} e^{2\pi(\frac{2}{9})^{\frac{3}{2}} j^{-\frac{1}{2}}} \right| \leq \frac{5}{1024\sqrt{2}} (4j+3) e^{\frac{16}{27} \pi j^{-\frac{1}{2}}}. \quad (96)$$

Using [1, 10.4.61 and 10.4.66], (91) and (93),

$$\left| (Ai'Bi')(-\tilde{a}_{j+1} + c_{2j}) - \left(-\frac{1}{2\pi} \left(\frac{2}{9} \right)^{\frac{1}{2}} \left(\frac{3\pi}{2} \right)^{\frac{1}{3}} j^{-\frac{1}{6}} \right) \right| \leq \frac{7}{768\sqrt{2}} \left(\frac{3\pi}{2} \right)^{\frac{1}{3}} j^{-\frac{1}{6}} (4j+3). \quad (97)$$

Using [1, 10.4.61], (91), (92) and (93),

$$\left| (Ai'(-\tilde{a}_{j+1} + c_{2j}))^2 - \frac{1}{4\pi} \left(\frac{2}{9} \right)^{\frac{1}{2}} \left(\frac{3\pi}{2} \right)^{\frac{1}{3}} j^{-\frac{1}{6}} e^{-2\pi(\frac{2}{9})^{\frac{3}{2}} j^{-\frac{1}{2}}} \right| \leq \frac{7}{1536} \left(\frac{3\pi}{2} \right)^{\frac{1}{3}} j^{-\frac{1}{6}} (4j+3) e^{-\frac{1}{2\sqrt{2}(4j+3)}}. \quad (98)$$

Using [1, 10.4.59 and 10.4.63], (91) and (94),

$$\left| (AiBi)(-\tilde{a}_{j+1} + c_{2j}) - \frac{1}{2\pi} \left(\frac{2}{9} \right)^{-\frac{1}{2}} \left(\frac{3\pi}{2} \right)^{-\frac{1}{3}} j^{\frac{1}{6}} \right| \leq \frac{5}{192} \left(\frac{3\pi}{8} (4j+3) \right)^{\frac{4}{3}}. \quad (99)$$

Finally, using [1, 10.4.59], (91), (92) and (94),

$$\left| (Ai(-\tilde{a}_{j+1} + c_{2j}))^2 - \frac{1}{4\pi} \left(\frac{2}{9} \right)^{-\frac{1}{2}} \left(\frac{3\pi}{2} \right)^{-\frac{1}{3}} j^{\frac{1}{6}} e^{-2\pi(\frac{2}{9})^{\frac{3}{2}} j^{-\frac{1}{2}}} \right| \leq \frac{5}{768} \frac{1}{\pi} \left(\frac{3\pi}{8} (4j+3) \right)^{\frac{4}{3}} e^{-\frac{1}{2\sqrt{2}(4j+3)}}. \quad (100)$$

With (86), (88), (89) and (95) we estimate (79). With (86), (87) and (96) we estimate (80). With (87) and (88) we estimate (81). With (87), (89) and (97) we estimate (82). With (88), (89) and (98) we estimate (83). With (90), (87), (89) and (99) we estimate (84). At last, with (90), (88), (89) and (100) we estimate (85). After straightforward but tedious computations, we obtain, for every $j \geq 1$ and for $c = c_{2j}$,

$$\begin{aligned} & \left| h(-\tilde{a}_{j+1}) - \left(1 + \frac{3\pi}{8} (4j+3) e^{2\pi(\frac{2}{9})^{\frac{3}{2}} j^{-\frac{1}{2}}} - \frac{3\pi}{32} (4j+3) \left(1 - \frac{9}{4} \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{7}{2}} \right) e^{-2\pi(\frac{2}{9})^{\frac{3}{2}} j^{-\frac{1}{2}}} \right. \right. \\ & \quad \left. \left. + \frac{5}{8} \left(\frac{2}{9} \right)^{\frac{1}{2}} \left(\frac{3\pi}{2} \right)^{\frac{1}{3}} j^{-\frac{1}{6}} \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{35}{24}} e^{-2\pi(\frac{2}{9})^{\frac{3}{2}} j^{-\frac{1}{2}}} \right) \right| \\ & \leq \pi \left(\left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{14}{3}} \frac{8}{3\pi} e^{-\frac{1}{2\sqrt{2}}(4j+3)^{-1}} \left(\frac{5}{48} \left(\frac{385}{4608} \right)^2 + \left(\frac{7315}{663552} \right)^2 \right) \frac{5}{1024\sqrt{2}} \right. \\ & \quad + \left(\frac{3\pi}{8} (4j+3) \right)^{-4} \frac{8}{3\pi} e^{\frac{16}{27}\pi j^{-\frac{1}{2}}} \left(\frac{5}{48} \right)^3 \frac{5}{1024\sqrt{2}} + \frac{1}{\pi} \left(\frac{3\pi}{8} (4j+3) \right)^{-4} \frac{5}{48} \frac{385}{4608} \\ & \quad + \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{11}{3}} j^{-\frac{1}{6}} \frac{5}{48} \frac{7315}{663552} \frac{7}{768\sqrt{2}} \frac{8}{3\pi} \left(\frac{3\pi}{2} \right)^{\frac{1}{3}} \\ & \quad + \left(\frac{3\pi}{8} (4j+3) \right)^{-4} j^{-\frac{1}{6}} e^{-\frac{1}{2\sqrt{2}}(4j+3)^{-1}} \frac{385}{4608} \frac{7315}{663552} \frac{7}{1536} \frac{8}{3\pi} \left(\frac{3\pi}{2} \right)^{\frac{1}{3}} \\ & \quad \left. + \left(\frac{3\pi}{8} (4j+3) \right)^{-4} \frac{5}{24} \frac{7315}{663552} \frac{5}{192} + \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{13}{3}} e^{-\frac{1}{2\sqrt{2}}(4j+3)^{-1}} \frac{2}{\pi} \frac{385}{4608} \frac{7315}{663552} \frac{5}{768} \right). \quad (101) \end{aligned}$$

In the upper bound of (101), the dominant term is, for every $j \geq 1$, $\frac{1}{\pi} \left(\frac{3\pi}{8} (4j+3) \right)^{-4} \frac{5}{48} \frac{385}{4608}$. Since $\frac{5}{48} \frac{385}{4608} \leq 9 \times 10^{-3}$, one finally obtains the less precise but sufficient estimate :

$$\begin{aligned} & \left| h(-\tilde{a}_{j+1}) - \left(1 + \frac{3\pi}{8} (4j+3) e^{2\pi(\frac{2}{9})^{\frac{3}{2}} j^{-\frac{1}{2}}} - \frac{3\pi}{32} (4j+3) \left(1 - \frac{9}{4} \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{7}{2}} \right) e^{-2\pi(\frac{2}{9})^{\frac{3}{2}} j^{-\frac{1}{2}}} \right. \right. \\ & \quad \left. \left. + \frac{5}{8} \left(\frac{2}{9} \right)^{\frac{1}{2}} \left(\frac{3\pi}{2} \right)^{\frac{1}{3}} j^{-\frac{1}{6}} \left(\frac{3\pi}{8} (4j+3) \right)^{-\frac{35}{24}} e^{-2\pi(\frac{2}{9})^{\frac{3}{2}} j^{-\frac{1}{2}}} \right) \right| \\ & \leq 7 \times 9 \times 10^{-3} \left(\frac{3\pi}{8} (4j+3) \right)^{-4}. \quad (102) \end{aligned}$$

The approximation of $h(-\tilde{a}_{j+1})$ in (102) is increasing in j and is approximately equal to 15.87 for $j = 1$, hence for every $j \geq 1$,

$$h(-\tilde{a}_{j+1}) \geq 15.87 - 6.3 \times 10^{-2} \times \left(\frac{3\pi}{8}(4j+3) \right)^{-4} > 0. \quad (103)$$

We prove that h remains strictly positive on the spectral band $[Y_{\max}^{2j}, Y_{\min}^{2j}]$. Recall that the spectral bands of \mathbf{H} are exponentially small. More precisely, [2, Theorem 2.5] implies that, for every $c \geq c_{2j}$,

$$[Y_{\max}^{2j}, Y_{\min}^{2j}] \subset [-\tilde{a}_{j+1} - \Lambda_{2j,c}, -\tilde{a}_{j+1} + \Lambda_{2j,c}]. \quad (104)$$

where

$$\Lambda_{2j,c} := \left(\frac{(Bi'(-\tilde{a}_{j+1}))^2}{2\pi\tilde{a}_{j+1}} + \frac{K_{2j}}{(c - \tilde{a}_{j+1})^{\frac{3}{2}}} \right) e^{-\frac{4}{3}(c - \tilde{a}_{j+1})^{\frac{3}{2}}} \quad (105)$$

and where we used the relationships $u'(-\tilde{a}_{j+1}) = -Ai'(0)Bi'(-\tilde{a}_{j+1})$ and $Ai(0)Ai'(0) = -\frac{1}{2\pi\sqrt{3}}$. Note that the notations in [2] and in the present paper correspond through $c = h^{-\frac{2}{3}}$. The constant K_{2j} is defined in the proof of [2, Proposition 6.1], but it can be much improved for our purpose. Indeed, using the notations given in this proof, one can actually set, for every $\tau > 0$,

$$B_{2j,\tau} := \sqrt{3}e^{\frac{2}{3}\tau - \frac{1}{2}(c_{2j} - \tilde{a}_{j+1})^2} (1 + 2.83\sqrt{3}\tau^{-\frac{3}{2}})$$

instead of

$$B_{2j,\tau} := \sqrt{3}e^{\frac{2}{3}\tau - \frac{1}{2}\tilde{a}_{j+1}^2} (1 + 2.83\sqrt{3}\tau^{-\frac{3}{2}}).$$

Indeed, similar to [2, (4.3) or (4.22)], one actually set $X = -X_{\max}^{2j} - h^{-\frac{2}{3}} + \tilde{a}_{j+1} \in [-c_{2j} + \tilde{a}_{j+1}, 0)$ which gives the good estimate corresponding to [2, (4.11)].

Following the proof of [2, Proposition 6.1] and using (90), we get that, for $\tau = c_{2j} - \tilde{a}_{j+1}$,

$$\forall j \geq 1, |K_{2j}| \leq 2 \times 10^6 \times j^{-\frac{11}{6}} e^{4\pi(\frac{2}{9})^{\frac{3}{2}}j^{-\frac{1}{2}}}. \quad (106)$$

Thus, using (86) and (89), for every $j \geq 1$,

$$\begin{aligned} \left| \frac{(Bi'(-\tilde{a}_{j+1}))^2}{2\pi\tilde{a}_{j+1}} + \frac{K_{2j}}{(c_{2j} - \tilde{a}_{j+1})^{\frac{3}{2}}} \right| &\leq \frac{9}{2} \frac{1}{\pi^2} \left(\frac{3\pi}{8}(4j+3) \right)^{-\frac{19}{6}} + 2 \times 10^6 \times j^{-\frac{11}{6}} e^{4\pi(\frac{2}{9})^{\frac{3}{2}}j^{-\frac{1}{2}}}. \\ &\leq 3 \times 10^6 \times j^{-\frac{11}{6}} e^{4\pi(\frac{2}{9})^{\frac{3}{2}}j^{-\frac{1}{2}}}. \end{aligned} \quad (107)$$

Hence, using (93), for every $j \geq 1$,

$$|\Lambda_{2j,c_{2j}}| \leq 3 \times 10^6 \times j^{-\frac{11}{6}} e^{4\pi(\frac{2}{9})^{\frac{3}{2}}j^{-\frac{1}{2}} - \frac{1}{2\sqrt{2}}(4j+3)^{-1}}. \quad (108)$$

Let $t \in [-1, 1]$. Since h is C^1 , by the Mean Value Theorem, for every $j \geq 1$ and every $c \geq c_{2j}$,

$$|h(-\tilde{a}_{j+1} + t\Lambda_{2j,c}) - h(-\tilde{a}_{j+1})| \leq \left(\sup_{y \in [Y_{\max}^{2j}, Y_{\min}^{2j}]} \left| \frac{dh}{dy}(y) \right| \right) \times |\Lambda_{2j,c}| \quad (109)$$

But, using (54), (55), (56) and (57), for every y ,

$$\begin{aligned} \frac{dh}{dy}(y) &= 2(2y+c)(UV' + VU')(y+c) - ((U'(y+c))^2 + (y+c)U(y+c)) \\ &\quad - 2y((V'(y+c))^2 + (y+c)V(y+c)) + (V(U-V'))(y+c). \end{aligned} \quad (110)$$

Using [1, 10.4.3, 10.4.63, 10.4.66], if $\eta > 0$ is any real number,

$$\forall x \geq \left(\frac{Ai'(0)}{Ai(0)} \right)^2 \eta^{-2}, \quad 0 \leq Bi'(x) \leq \eta x^{\frac{1}{2}} Bi(x). \quad (111)$$

Since for any $x \geq 0$, $Ai(x) \leq Bi'(x)$ and $|Ai'(x)| \leq Bi'(x)$, using the expressions of u and v in terms of Airy functions leads to, for any real number $\eta > 0$ and any $y \in [-c, 0]$,

$$y + c \geq \left(\frac{Ai'(0)}{Ai(0)} \right)^2 \eta^{-2} \Rightarrow |U'(y + c)| \leq \eta(y + c)^{\frac{1}{2}} |U(y + c)| \quad (112)$$

$$\text{and } y + c \geq \left(\frac{Ai'(0)}{Ai(0)} \right)^2 \eta^{-2} \Rightarrow |V'(y + c)| \leq \eta(y + c)^{\frac{1}{2}} |V(y + c)|. \quad (113)$$

Moreover, for every $y \in [-c, 0]$,

$$|U(y + c)| \leq 2|U'(y + c)| \quad (114)$$

and

$$|V(y + c)| \leq 2|V'(y + c)|. \quad (115)$$

If $y \in [Y_{\max}^{2j}, Y_{\min}^{2j}]$, then $y + c \geq Y_{\max}^{2j} + c$. Hence, using (112) and (113) with $\eta = \left(\frac{Ai'(0)}{Ai(0)} \right)^{\frac{1}{2}} (Y_{\max}^{2j} + c)^{-\frac{1}{2}}$ and using (114) and (115),

$$\sup_{y \in [Y_{\max}^{2j}, Y_{\min}^{2j}]} \left| \frac{dh}{dy}(y) \right| \leq 6 \left(\frac{Ai'(0)}{Ai(0)} \right)^{\frac{1}{2}} (Y_{\max}^{2j} + c)^{-\frac{1}{2}} (Y_{\min}^{2j} + c)^{\frac{3}{2}} \sup_{y \in [Y_{\max}^{2j}, Y_{\min}^{2j}]} |h(y)| \quad (116)$$

Combining (102), (103), (108), (109) and (116), one gets that (for $c = c_{2j}$), for every $j \geq 1$ and every $t \in [-1, 1]$, $h(-\tilde{a}_{j+1} + t\Lambda_{2j, c_{2j}}) > 0$. Therefore, for every $c \geq c_{2j}$, every $j \geq 1$ and every $t \in [-1, 1]$, $h(-\tilde{a}_{j+1} + t\Lambda_{2j, c}) > 0$. By (104), it leads to $h(y) > 0$ for every $y \in [Y_{\max}^{2j}, Y_{\min}^{2j}]$. This proves Lemma 1.

Remark. With (104), (105) and (109) it is easy to show that for c arbitrary large, the result of Lemma 1 is true. What is difficult here is to be able to take c only larger than c_{2j} .

APPENDIX C. THE CASE OF AN EVEN NUMBER OF WELLS

All the results remain true in the case of an even number of potential wells. Slight changes have to be made in order to carry on the proofs done in the odd case. First, we have to define the potential corresponding to an even number $2N$ of wells in a way that the potential function is an even function.

$$V_{2N} : x \mapsto \sum_{k=-N+1}^N V(x - 2kL_0 + L_0) \quad (117)$$

where V is defined in (3). After rescaling as in the odd case, we consider

$$\mathbf{V}_{2N} : z \mapsto \sum_{k=-N+1}^N \mathbf{V}(z - 2k + 1)$$

Then, instead of defining the functions U and V as in (13) and (14), we set :

$$U(x) = v'(-\mathbf{E})u(x) - u'(-\mathbf{E})v(x)$$

and

$$V(x) = u(-\mathbf{E})v(x) - v(-\mathbf{E})u(x).$$

The parity of the number of wells played a role in the proof of the absence of eigenvalues in the spectral gaps of \mathbf{H} . Following the proof of Section 3.3.1, there is no change to do in the first case. In the second case, corresponding to the spectral gaps $(Y_{\min}^{4j+3}, Y_{\max}^{4j+2})$ or $(Y_{\min}^{4j+1}, Y_{\max}^{4j})$, one has still $a + b < 0$ and $a - b < 0$, but now $(a + b)^{2N} > 0$ and $(a - b)^{2N} > 0$. Thus, the first term in (40) is strictly positive. For the second term, since $a - b < a + b < 0$

we have $(a - b)^{2N} > (a + b)^{2N}$ and the second term in (40) is now strictly negative. In particular, it does not vanish on these spectral gaps and thus H_{2N} has no eigenvalues in the spectral gaps of H .

In the other proofs, the parity of the number of wells does not play any role. Our choice of focusing on an odd number of wells was guided by the fact that it is naturally involved in the definition of the integrated density of states.

REFERENCES

- [1] M.A. Abramovitz, I.A. Stegun, *Handbook for mathematical functions with formulas, graphs, and mathematical tables*, 9th edition, Applied Mathematics Series **55**, Washington D.C. (1990).
- [2] H. Boumaza, O. Lafitte, *The band spectrum of the periodic Airy-Schrödinger operator on the real line*, J. Differential Equations **264**(1), 455-505 (2018), DOI:10.1016/j.jde.2017.09.013
- [3] R. Carmona, J. Lacroix, *Spectral Theory of Random Schrödinger Operators*, Probability and Its Applications. Birkhauser, Boston, 1990.
- [4] Y.Q. Gao et al., *On the theory of electron transfer reactions at semiconductor electrode liquid interfaces*, Journal of chemical physics **112**(7), 3358-3369 (2000).
- [5] B. Helffer, J. Sjöstrand, *Multiple wells in the semiclassical limit. I.*, Comm. Partial Differential Equations **9**(4), 337-408 (1984).
- [6] V. Ivrii, *Complete semiclassical spectral asymptotics for periodic and almost periodic perturbations of constant operators*, arXiv:1808.01619
- [7] Y. E. Karpeshina, *On the density of states for the periodic Schrödinger operator*, Ark. Mat. **38**(1), 111-137 (2000).
- [8] S. Kar, *Effect of Out-Tunneling Leakage and Electron-Hole Asymmetry on Modulation Response of Semiconductor Double Tunneling-Injection Quantum Dot Lasers*, Master Thesis, Virginia Polytech Institute and State University.
- [9] W. Kirsch, B. Metzger, *The integrated density of states for random Schrödinger operators*. Spectral theory and mathematical physics: a Festschrift in honor of Barry Simon's 60th birthday, 649-696, Proc. Sympos. Pure Math., **76**(2), Amer. Math. Soc., Providence, RI, 2007.
- [10] V. Kostrykin, R. Schrader, *Global bounds for the Lyapunov exponent and the integrated density of states of random Schrödinger operators in one dimension*. J. Phys. A **33**(46), 8231-8240 (2000).
- [11] S. Kotani, B. Simon, *Stochastic Schrödinger operators and Jacobi Matrices on the Strip*, Commun. Math. Phys. **119**(3), 403-429 (1988).
- [12] W. Lui, M. Fukuma, *Exact solution of the Schrödinger equation across an arbitrary one-dimensional piecewise-linear potential barrier*, Journal of Applied Physics **60**, 1555 (1986).
- [13] L. Parnowski, R. Shterenberg, *Asymptotic expansion of the integrated density of states of a two-dimensional periodic Schrödinger operator*, Invent. Math. **176**(2), 275-323 (2009).
- [14] L. Qi, *Formula for the IDS of periodic Jacobi matrices*, arXiv:1808.09084
- [15] M. Reed, B. Simon, *Methods of Modern Mathematical Physics IV: Analysis of operators*, Academic Press, New York, (1978).
- [16] D. Shenk, M. A. Shubin, *Asymptotic expansion of the spectral function of the Hill operator*, (Russian) Funktsional. Anal. i Prilozhen. **20**(1), 89-90 (1986).
- [17] A. V. Sobolev, *Asymptotics of the integrated density of states for periodic elliptic pseudo-differential operators in dimension one*, Rev. Mat. Iberoam. **22**(1), 55-92 (2006).
- [18] D. R. Yafaev, *Passage through a potential barrier and multiple wells*, St. Petersburg Math. J. **29**(2), 399-422 (2018).
- [19] J.-P. Yang et al., *Fermi-level pinning appears upon weak electrode-organic contact without gap states: A universal phenomenon*, Organic Electronics **48**, 172-178 (2017).

H. BOUMAZA, UNIVERSITÉ SORBONNE PARIS NORD, LAGA, CNRS, UMR 7539, F-93430, VILLETANEUSE, FRANCE

E-mail address: boumaza@math.univ-paris13.fr

O. LAFITTE, UNIVERSITÉ SORBONNE PARIS NORD, LAGA, CNRS, UMR 7539, F-93430, VILLETANEUSE, FRANCE

UNIVERSITÉ DE MONTRÉAL, CRM, UMI 3457, MONTRÉAL, QUÉBEC, CANADA

E-mail address: lafitte@math.univ-paris13.fr