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# THE BAND SPECTRUM OF THE PERIODIC AIRY-SCHRÖDINGER OPERATOR ON THE REAL LINE

H. BOUMAZA AND O. LAFITTE

*A tribute to Louis Boutet de Monvel (1941-2014)*

ABSTRACT. We introduce the periodic Airy-Schrödinger operator and we study its band spectrum. This is an example of an explicitly solvable model with a periodic potential which is not differentiable at its minima and maxima. We define a “classical regime”, a “semiclassical regime” and a “semiclassical limit”. We prove that there exists an explicit constant, which is a zero of a classical function, which marks the transition between the classical and semiclassical regimes. We completely determine the behaviour of the edges of the first spectral band with respect to our semiclassical parameter. Then, we investigate the spectral bands situated in the range of the potential. In the semiclassical regime, we prove precise estimates on the widths of the spectral bands and the spectral gaps and we determine an upper bound on the spectral density in this range. Finally, in the semiclassical limit, we get asymptotics expansions of the edges of the spectral bands and thus of the widths of the spectral bands and the spectral gaps.

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## 1. THE MODEL, ITS CANONICAL SOLUTIONS AND THE SEMICLASSICAL PARAMETER

**1.1. The periodic Airy-Schrödinger operator.** Let  $2L_0 \in \mathbb{R}_+^*$  be a characteristic length modelling the distance between two ions in a one dimensional periodic lattice of ions. The motion of electrons in this lattice can be studied through the following  $2L_0$ -periodic Schrödinger operator acting on the Sobolev space  $H^2(\mathbb{R})$ ,

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V, \quad (1)$$

where  $V$  is the  $2L_0$ -periodic function on  $\mathbb{R}$  defined by

$$\forall x \in [-L_0, L_0], \quad V(x) = V_0 \left( \frac{|x|}{L_0} - 1 \right),$$

$V_0 \in \mathbb{R}_+^*$  being a reference potential. The ions, in this model, are located at points  $2nL_0$  for  $n \in \mathbb{Z}$ , this points corresponding to the minima of the potential  $V$ .

A first important observation is that  $V$  is not differentiable on its minima and maxima points.

We call  $H$  the *periodic Airy-Schrödinger operator* on  $\mathbb{R}$ .

The classical theory (Reed and Simon, [26]) asserts that the operator  $H$ , like any periodic operator, has purely absolutely continuous spectrum and that this spectrum is the union of spectral bands:

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

where  $E_{\min}^p$  and  $E_{\max}^p$  are the spectral band edges and the intervals  $(E_{\max}^p, E_{\min}^{p+1})$  are the spectral gaps. We will precise these notations and characterize these spectral band edges in Section 3.

A classical analysis is the calculation of the bands near the minimum of the potential,  $-V_0$ . We will describe, more precisely, the bands whose intersection with the range of  $V$  is not empty. We are able to count the number of spectral bands in  $[-V_0, 0]$ , the range of the potential  $V$ , for any value of a dimensionless parameter defined in (4), and to describe precisely these spectral bands.

1.2. **The semiclassical parameter.** As  $V$  is continuous and bounded, a solution  $\psi$  of the equation:

$$-\frac{\hbar^2}{2m}\psi'' + V(x)\psi = E\psi \quad (2)$$

satisfies  $\psi \in C^1(\mathbb{R})$ .

A crucial remark is the following: as  $V'$  is piecewise constant, in our case  $V'(x) = \pm \frac{V_0}{L_0}$  for all  $x \notin L_0\mathbb{Z}$ , one recognizes in (2), after rescaling, the celebrated Airy equation :  $u'' = xu$ .

On the interval  $[0, L_0]$ , the rescaling is done through a parameter  $\theta$  given as the unique real number such that

$$-\frac{\hbar^2}{2m}\theta^2 \frac{V_0^2}{L_0^2}(\theta(V(x) - E)) + V(x) - E = 0,$$

namely

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

Note that  $\theta V(x)$  is dimensionless for all values of  $x \in \mathbb{R}$  and thus we introduce our dimensionless semiclassical parameter:

$$\theta V_0 = \left( \frac{2mL_0^2 V_0}{\hbar^2} \right)^{\frac{1}{3}}. \quad (4)$$

This semiclassical parameter  $\theta V_0$  allows to define different types of regimes and limits in which we study the spectral properties of the periodic Airy-Schrödinger operator. Recall that the range of the potential  $V$  is the interval  $[-V_0, 0]$ .

**Definition 1.** *The operator  $H$  is said to be:*

- (1) *in the **semiclassical limit** when the semiclassical parameter  $\theta V_0$  tends to infinity ;*
- (2) *in the **semiclassical regime** when there exists  $E \in [E_{\min}^0, 0]$  such that  $E \notin \sigma(H)$  ;*
- (3) *in the **classical limit** when the semiclassical parameter  $\theta V_0$  tends to 0 ;*
- (4) *in the **classical regime** when  $\sigma(H) \cap [-V_0, 0] = [E_{\min}^0, 0]$ .*

Note that this definition of the semiclassical limit corresponds to the usual semiclassical limit for which “ $\hbar$  tends to 0”, since  $\theta V_0$  and  $\hbar$  satisfy (4).

For any  $E > -V_0$ , an electron admits a classical trajectory which is solution of the ordinary differential equation  $\frac{1}{2}m\dot{x}^2 + V(x) = E$  (see [2]). In the classical regime, the equation (2) also has a non-trivial solution for any  $E \in [E_{\min}^0, 0]$ . This solution corresponds to an electron which scatters through the lattice since the spectrum of  $H$  is absolutely continuous. Although the classical trajectory of this electron is trapped (since  $E \leq 0$ ), the tunneling effect allows the quantum diffusion of the electron.

In the semiclassical regime, there exists an energy  $E \in [E_{\min}^0, 0]$  which lies in a spectral gap of  $H$ . For this “forbidden” energy, one could still have solutions of (2), but these solutions are no longer in  $H^2(\mathbb{R})$  and not even in  $L^2(\mathbb{R})$ . To be able to

interpret these solutions as probability densities of presence of a particle, one need to perform a cut-off localized closely to a minimum of the potential. It leads to the existence of quantum trapped modes for which there is no quantum diffusion since there is no tunneling effect.

In the classical regime there is quantum diffusion at every energy in the range of the potential while in this range, in the semiclassical limit, there is no longer any quantum diffusion and there remain only trapped modes (Corollary 2 and Appendix C). Since the semiclassical regime marks the appearance of some trapped mode in the range of the potential, it is an intermediate regime between the classical one and the semiclassical limit.

Differences between the classical regime and the quantum regime are discussed through two examples in [24]. For general references about semiclassical analysis we refer to the textbooks [8, 18, 30].

We use the semiclassical parameter  $\theta V_0$  to rewrite the periodic Airy-Schrödinger operator in two different forms which recall operators studied in the classical literature ([13, 19]). If  $f$  is a function defined on an interval  $I$  of length  $T$ , let  $f^{\#T}$  be the periodic function of period  $T$  which coincide with  $f$  on  $T$ . Then, the equation (2) is equivalent to

$$-\frac{d^2}{dx^2}\psi + (|x + \theta V_0| - \theta V_0)^{\#(2\theta V_0)}\psi = \theta E\psi \quad (5)$$

or

$$-h^2 \frac{d^2}{dz^2}\phi + (|z + 1| - 1)^{\#2}\phi = \frac{\theta E}{\theta V_0}\phi \quad \text{with } h = (\theta V_0)^{-\frac{1}{3}}. \quad (6)$$

We will study in the sequel two different cases:  $-\theta E$  bounded and  $\theta V_0$  tends to infinity for the first case and  $-\theta V_0 - \theta E$  bounded and  $\theta V_0$  tends to infinity for the second one. The first case studies the spectrum of  $H$  near the maximum of the potential  $V$  and corresponds to [19]. The second case is the study of the bottom of the spectrum and corresponds to [13].

Our study of the semiclassical regime of the periodic Airy-Schrödinger operator was first motivated by giving a rigorous treatment of the numerical results in [5], a paper which deals with the question of quark confinement. It was also motivated by previous results of one of the authors on the semiclassical analysis of the Rayleigh-Taylor instability [7, 14, 17]. Note that the periodic Airy-Schrödinger model is also closely related with an infinite periodized sawtooth junction PN in photonic crystals, giving an explicitly solvable situation in a quantum setting (see [20]).

After a thorough study of the periodic Airy-Schrödinger operator, we deduced that this model gives, up to our knowledge, a first example of an operator for which one can give an explicit value of the semiclassical parameter for which a transition between the classical and the semiclassical regimes occurs. This special value of the semiclassical parameter is characterized as a zero of the derivative of one of the canonical solution of the Airy equation. Moreover, we identified a sequence of values of this semiclassical parameter which counts the number of bands in the range of the potential.

**1.3. The canonical solutions of the Airy equation.** Let  $u$  and  $v$  be 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. The Airy function  $Ai$  plays a very special role for the ordinary differential equation  $u'' = xu$ . It generates the unique family of subdominant solutions of this Sturmian equation. It is also the unique solution of the Airy equation which is in  $\mathcal{S}'(\mathbb{R})$  and such that  $\widehat{Ai}(0) = 1$ . The function  $Bi$  is the solution of the Airy equation satisfying the initial conditions  $Bi(0) = \sqrt{3}Ai(0)$  and  $Bi'(0) = -\sqrt{3}Ai'(0)$ . One has the expression of  $u$  and  $v$  in terms of the classical Airy functions  $Ai$  and  $Bi$ :

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

and

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

Both  $u$  and  $v$  are analytic functions on  $\mathbb{R}$ . Moreover,  $u$  is strictly decreasing and negative on  $[0, +\infty[$  and  $v$  is strictly increasing and positive on  $(0, +\infty)$ . Thus, the zeroes of  $u$ ,  $v$  and their derivatives are all non-positive real numbers.

**Notation.** We denote by

- $\{-\tilde{c}_{2j}\}_{j \geq 0}$  the set of the zeroes of  $u$ ,
- $\{-\tilde{c}_{2j+1}\}_{j \geq 0} \cup \{0\}$  the set of the zeroes of  $u'$ ,
- $\{-c_{2j+1}\}_{j \geq 0} \cup \{0\}$  the set of the zeroes of  $v$ ,
- $\{-c_{2j}\}_{j \geq 0}$  the set of the zeroes of  $v'$ .

This definition is precised in Section 4.2.

An important property of these zeroes, which is proven in Corollary 3, is:

$$\forall k \geq 0, \quad -\tilde{c}_k < -c_k.$$

Approximate values of the  $c_k$  and  $\tilde{c}_k$  can be given. For example,

$$c_0 \simeq 1.515, \quad \tilde{c}_0 \simeq 1.986, \quad c_1 \simeq 2.666, \quad \tilde{c}_1 \simeq 2.948.$$

## 2. MAIN RESULTS

**2.1. The first spectral band in the classical and semiclassical regimes.** For the parameter  $\theta V_0$ , the value  $c_0$  marks the transition between two different regimes of the system: the classical and the semiclassical regimes. The following result gives a precise version of this statement.

**Theorem 1.** *For  $\theta V_0 \leq c_0$ , the only gap in  $[-V_0, 0]$  is the "ground state gap"  $[-V_0, E_{\min}^0]$ . The first non trivial gap intersects  $[-V_0, 0]$  as soon as  $\theta V_0 > c_0$ .*

Thus, the semiclassical regime is characterized by the inequality  $\frac{1}{\theta V_0} < \frac{1}{c_0}$  while the classical regime is characterized by  $\frac{1}{\theta V_0} \geq \frac{1}{c_0}$ .

Two  $\theta V_0$ -dependent integers are of interest in this paper:

(1) the unique integer  $p_0$  such that

$$\tilde{c}_{p_0+1} - \tilde{c}_{p_0} < \theta V_0 \leq \tilde{c}_{p_0} - \tilde{c}_{p_0-1} \quad \text{when} \quad \theta V_0 < c_0; \quad (7)$$

(2) the unique integer  $k_0$  such that

$$c_{k_0} < \theta V_0 < \tilde{c}_{k_0} \quad \text{or} \quad \tilde{c}_{k_0} < \theta V_0 < c_{k_0+1} \quad \text{when} \quad \theta V_0 > c_0. \quad (8)$$

The integers  $p_0$  and  $k_0$  determine the regions in which the spectral bands are, respectively in the classical and the semiclassical regimes.

In the classical limit, the first spectral band tends to cover all the interval  $[-\frac{V_0}{2}, +\infty)$ .

**Theorem 2.** *When  $V_0$  is fixed,*

$$\lim_{\theta \rightarrow 0} E_{\min}^0 = -\frac{V_0}{2} \quad \text{and} \quad \lim_{\theta \rightarrow 0} E_{\max}^0 = +\infty.$$

One can actually get much more precise estimates of the rescaled ground state  $\theta E_{\min}^0$  in both classical and semiclassical regimes. Before stating them, we need to introduce notations for the zeroes of the Airy function  $Ai$  and its derivative.

**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  $(-\infty, 0]$ . Moreover, for every  $j \geq 1$ ,  $-a_j \in (-\tilde{a}_{j+1}, -\tilde{a}_j)$ .

We set  $\alpha = -\frac{Ai(0)}{Ai'(0)} > 0$ . The number  $\alpha$  is the inverse of the slope at 0 of the Airy function  $Ai$ . An approximate value of  $\alpha$  is:  $\alpha \simeq 1,372$ .

**Theorem 3.** *We have the following estimates on  $\theta E_{\min}^0$ :*

(1) *For every  $\theta V_0 > 0$*

$$-\theta V_0 < \theta E_{\min}^0 < \min\left(-\frac{\theta V_0}{2}, -\theta V_0 + \tilde{a}_1\right). \quad (9)$$

(2) *When  $\theta V_0$  tends to  $+\infty$ ,*

$$\theta E_{\min}^0 = -\theta V_0 + \tilde{a}_1 - \alpha \sqrt{3} \frac{(u'(-\tilde{a}_1))^2}{\tilde{a}_1} e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_1)^{\frac{3}{2}}} \left(1 + \mathcal{O}\left((\theta V_0 - \tilde{a}_1)^{-\frac{3}{2}}\right)\right).$$

(3) *When  $\theta V_0$  tends to 0,*

$$\theta E_{\min}^0 = -\frac{\theta V_0}{2} - \frac{1}{120}(\theta V_0)^4 + \mathcal{O}((\theta V_0)^7). \quad (10)$$

The proof of this Theorem is described in Section 6.2.

**Remark.** The value  $-\frac{V_0}{2}$  which appears in the last point is the mean value of the periodic potential  $V$ .

**2.2. An associated multidimensional model.** Let  $d \geq 1$  an integer. The results on  $E_{\min}^0$  give us a precise description of the spectrum of the following periodic operator on  $\mathbb{R}^d$  associated to  $H$ :

$$H_d = -\frac{\hbar^2}{2m} \Delta_d + V_d \quad \text{acting on} \quad \mathbf{H}^2(\mathbb{R}^d), \quad (11)$$

where  $\Delta_d$  is the Laplacian on  $\mathbb{R}^d$  and  $V_d$  is the maximal multiplication operator by the function defined by

$$\forall (x_1, \dots, x_d) \in \mathbb{R}^d, V_d(x_1, \dots, x_d) = V(x_1).$$

**Proposition 1.** *If  $\sigma_{\text{ac}}(H_d)$  denote the absolutely continuous spectrum of  $H_d$ , then*

$$\sigma(H_d) = \sigma_{\text{ac}}(H_d) = [E_{\min}^0, +\infty).$$

Since  $\sigma(H_d)$  depends only on  $E_{\min}^0$ , Theorem 3 gives us a complete description of the behaviour of this spectrum with respect to  $\theta V_0$ .

**2.3. Spectral bands in the range of  $V$  in the semiclassical regime.** We have estimates on the widths of the spectral bands and the spectral gaps which are located in the range of  $V$ .

Let  $p \geq 0$  an integer and denote by  $\delta_p$  the width of the  $p$ -th spectral band and by  $\gamma_p$  the width of the  $p$ -th spectral gap with  $\delta_p = E_{\max}^p - E_{\min}^p$  and  $\gamma_p = E_{\min}^{p+1} - E_{\max}^p$ .

Let  $I$  be the strictly decreasing function defined on  $[1, +\infty)$  by

$$\forall y \geq 1, I(y) = \left(\frac{9}{4}\right)^{\frac{2}{3}} \frac{y^{\frac{3}{2}} + 1}{y^2 + y + 1}.$$

**Theorem 4.** *Let  $\theta V_0 > c_0$  and  $k_0$  introduced in (8).*

- (1) *The  $k_0$  first spectral bands are included in the range of  $V$ ,  $[-V_0, 0]$ .*
- (2) *One has, for every  $p \in \{2, \dots, k_0\}$ ,*

$$0 < \theta \delta_p \leq \left(\frac{\pi}{3} + \frac{7}{3\pi} \frac{p + \frac{1}{3}}{p(p + \frac{2}{3})}\right) \left(\frac{3}{\pi}\right)^{\frac{1}{3}} \frac{1}{p^{\frac{1}{3}}}, \quad (12)$$

*and for every  $p \in \{2, \dots, k_0 - 1\}$ ,*

$$0 < I\left(\left(\frac{7}{6}\right)^{\frac{2}{3}}\right) \frac{2^{\frac{1}{3}} \pi^{\frac{2}{3}}}{9} \frac{1}{(p+1)^{\frac{1}{3}}} < \theta \gamma_p \leq \left(\pi + \frac{7}{3\pi} \frac{p}{p^2 - 1}\right) \left(\frac{3}{\pi}\right)^{\frac{1}{3}} \frac{1}{(p-1)^{\frac{1}{3}}}. \quad (13)$$

*In particular, all the gaps in  $\sigma(H)$  are open.*

Note that we do not have a lower bound of  $\theta \delta_p$ . A still open conjecture is whether or not  $\theta \delta_p$  has an exponential lower bound.

The fact that all the gaps are open is also a consequence of general results which states that the potentials for which one has a finite number of gaps are analytic functions (see [28] for references on the topic and a discussion of the results of Skriganov).

One cannot expect an upper bound in (13) which is smaller than any power of  $p$  since, by results of Hochstadt, it would imply that  $V$  is a smooth function (see [16]). Moreover, an exponentially small upper bound of  $\theta \gamma_p$  is characteristic from the analyticity of  $V$  (see [29]). For general results on singular potentials for the Hill equation, we refer to [9].

The inequality (12) implies an upper bound for the spectral density in the range of the potential  $V$  in the semiclassical limit. Let  $k_0(\theta V_0)$  be the integer defined in (8). For any  $\theta V_0 > c_0$  we denote by  $D_{\theta V_0}$  the sum of the lengths of the  $k_0(\theta V_0)$  first



rescaled spectral bands (which are all included in the range of  $\theta V$ ) divided by the length of the range of  $\theta V$ :

$$\forall \theta V_0 > c_0, D_{\theta V_0} = \frac{1}{\theta V_0} \sum_{p=2}^{k_0(\theta V_0)} \theta \delta_p.$$

**Corollary 1.** *When  $\theta V_0$  tends to infinity,  $D_{\theta V_0}$  admits a limit denoted by  $D_V$ . Moreover,*

$$0 < D_V \leq \left(\frac{2}{3}\right)^{\frac{1}{3}}. \quad (14)$$

The limit  $D_V$  can be interpreted as the spectral density in the range of the potential  $V$  in the semiclassical limit.

Note that the number of gaps intersecting  $[-V_0, 0]$  has a jump for the semiclassical parameter at any number of the sequence  $(c_k)_{k \geq 0}$ . To complete the first point of Theorem 4 we observe that the roots of the canonical solutions of the Airy equation and their derivatives characterize the values of the asymptotic parameter  $\theta V_0$  for which a spectral band either enters in the range of the potential  $[-V_0, 0]$  or completes its entrance:

**Theorem 5.** *There exists a unique spectral band for which either the upper or the lower edge is equal to 0 if and only if  $\theta V_0 \in \{c_p, \tilde{c}_p\}_{p \geq 0}$ .*

For any function  $f$ , let  $Z(f)$  denotes the set of the zeroes of  $f$ . Then, Theorem 5 implies that:

$$Z(\theta V_0 \mapsto \theta E_{\max}^p(\theta V_0)) = Z(v) \cup Z(v')$$

and

$$Z(\theta V_0 \mapsto \theta E_{\min}^{p+1}(\theta V_0)) = Z(u) \cup Z(u').$$

**2.4. Spectral bands and spectral gaps in the semiclassical limit.** Thanks to the explicit form of the bands, other asymptotic formulas can be proven.

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

**Theorem 6.** *Let  $p \geq 0$ . The rescaled and shifted  $p$ -th spectral band,*

$$[\theta V_0 + \theta E_{\min}^p, \theta V_0 + \theta E_{\max}^p]$$

*asymptotically approaches the value  $\mathbf{a}_p$ . Moreover, in the limit when  $\theta V_0$  tends to infinity, its width is,*

$$\theta \delta_{2j} = 2\alpha \sqrt{3} \frac{(u'(-\tilde{a}_{j+1}))^2}{\tilde{a}_{j+1}} e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_{j+1})^{\frac{3}{2}}} \left(1 + \mathcal{O}\left((\theta V_0 - \tilde{a}_{j+1})^{-\frac{3}{2}}\right)\right), \quad (15)$$

and

$$\theta \delta_{2j+1} = 2\alpha \sqrt{3} (u(-a_{j+1}))^2 e^{-\frac{4}{3}(\theta V_0 - a_{j+1})^{\frac{3}{2}}} \left(1 + \mathcal{O}\left((\theta V_0 - a_{j+1})^{-\frac{3}{2}}\right)\right). \quad (16)$$

The widths of two consecutive bands  $\theta\delta_{2j}$  and  $\theta\delta_{2j+1}$  are of the same order in  $j$  since

$$\frac{(u'(-\tilde{a}_{j+1}))^2}{\tilde{a}_{j+1}} = 4\pi(Ai'(0))^2(\tilde{a}_{j+1})^{-\frac{1}{2}} + \mathcal{O}\left((\tilde{a}_{j+1})^{-\frac{5}{2}}\right), \quad (17)$$

$$(u(-a_{j+1}))^2 = 4\pi(Ai'(0))^2(a_{j+1})^{-\frac{1}{2}} + \mathcal{O}\left((a_{j+1})^{-\frac{3}{2}}\right), \quad (18)$$

$\tilde{a}_{j+1} = \mathcal{O}\left(j^{\frac{2}{3}}\right)$  and  $a_{j+1} = \mathcal{O}\left(j^{\frac{2}{3}}\right)$ . Estimates (17) and (18) are proven in Section 4.1.

We can interpret the first statement of Theorem 6 as a convergence of the band spectrum of the periodic Airy-Schrödinger operator to the pure point spectrum of the Schrödinger operator for a linear potential well.

**Corollary 2.** *For every  $p \geq 0$ , the  $p$ -th rescaled spectral band of the periodic Airy-Schrödinger operator tends to the singleton  $\{\mathbf{a}_p\}$  when  $\theta V_0$  tends to  $+\infty$ .*

We prove this corollary in Appendix C.

Theorem 6 compares with the result of Harrell [13, Theorem 1.1], since  $-2\text{Re} \int_0^{\theta V_0} |x - a_{j+1}|^{\frac{1}{2}} dx = -\frac{4}{3}(\theta V_0 - a_{j+1})^{\frac{3}{2}}$  (and the same expression with  $\tilde{a}_{j+1}$  instead of  $a_{j+1}$ ). Indeed, the operator studied by Harrel is the operator described in (5), where  $\theta V_0 = \frac{1}{\kappa}$ :

$$-\frac{d^2}{dx^2} + \kappa^{-2}q(\kappa x), \quad \kappa > 0,$$

acting on  $H^2(\mathbb{R})$ , where  $q$  is a potential which is periodic of period 2, having a non-degenerate smooth minimum at 0, is symmetric about 1 and its maximum value is positive.

In particular  $q$  is assumed to be at least two times differentiable at its minima and maxima points, thus our result is stated for a potential which satisfies weaker assumptions than those of Harrell since it is not even differentiable at its maxima and minima points.

Moreover, Harrel, for homotety reasons, assumes that  $q''(0) = \frac{1}{2}$ . The leading order term of the operator is thus

$$-\frac{d^2}{dx^2} + \frac{1}{2}x^2$$

and its spectrum is the classical spectrum of the harmonic oscillator  $\{2n + 1\}_{n \geq 0}$ . For results on the spectrum of the perturbed harmonic oscillator, one can read [3].

The asymptotic result of Harrel on the width of the spectral bands concerns thus the eigenvalues  $E$  close to a fixed odd number  $2n + 1$ , which corresponds to eigenvalues of  $-\frac{\hbar^2}{2m} \frac{d^2}{dy^2} + q(y)$  close to  $\frac{2n+1}{\sqrt{m}} \hbar$  (since  $q''(0) = \frac{1}{2}$ ), hence extremely close to the minimum of the potential. In our asymptotic results, this corresponds to  $\theta V_0$  tends to  $+\infty$ ,  $-\theta E$  tends to  $+\infty$  and  $\theta E + \theta V_0$  close to an eigenvalue of  $-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_0|x|$ , hence to the values in  $\{\mathbf{a}_p\}_{p \geq 0}$ .

The result of Harrel was later precised in [15] and generalized for the first spectral band in the multidimensional case (see [22, 27]).

The formulas (15) and (16) show that the rescaled spectral bands have exponentially small widths. On the contrary, the rescaled spectral gaps in the spectrum of  $H$  have constant widths.

**Theorem 7.** *When  $\theta V_0$  tends to  $+\infty$ , for every  $p \geq 0$ ,*

$$\theta \gamma_p = \mathfrak{a}_p - \mathfrak{a}_{p+1} + \mathcal{O}\left(e^{-\frac{4}{3}(\theta V_0 + \mathfrak{a}_{p+1})^{\frac{3}{2}}}\right). \quad (19)$$

More precise asymptotics for the width of the gaps can be found in Proposition 17.

The rescaled gaps have constant widths which are given by the differences between two consecutive zeroes of  $A_i$  and  $A_i'$ .

Theorems 6 and 7 are stated in the case where  $\theta V_0 + \theta E$  remains bounded and close to one of the  $\mathfrak{a}_p$  for  $p$  fixed, and  $\theta V_0$  tends to  $+\infty$ . It corresponds to looking at spectral bands and gaps close to the bottom of the potential,  $-V_0$ , and thus to the bottom of the spectrum in the semiclassical limit.

We can prove similar asymptotic expansions in the case where  $\theta E$  remains bounded and close to one of the  $\mathfrak{a}_p$  for  $p$  fixed, and  $\theta V_0 + \theta E$  tends to  $+\infty$ . This second case corresponds to energy bands close to the maximum of the potential. In this second case, we number the bands starting with the band of highest energy in  $[-V_0, 0]$ , labeled as the band 1 while the lowest band is labeled by  $k_0$  defined in (8).

Another case which can be dealt with, is when one assume that  $\theta E$  is closed to  $\frac{\mathfrak{a}_p}{(\theta V_0)^{\frac{1}{2}}}$  for some fixed  $p$  and there exists constants  $C_1 > 0$  and  $C_2 > 0$  such that  $\frac{\mathfrak{a}_p}{(\theta V_0)^{\frac{1}{2}}} \in [C_1, C_2]$ . In this case our bootstrap technique detailed in the proof of

Theorem 3 applies since  $e^{-\frac{4}{3}(\theta V_0 + \mathfrak{a}_p)^{\frac{3}{2}}} \cdot e^{\frac{4}{3}(\theta V_0)^{\frac{3}{2}}} \in [e^{C_1}, e^{C_2}]$ . This proves a result similar to Theorem 8.1 of März (in the case  $\mu \in [-Ch, 0]$  with the notations of [19]) for the widths of the gaps and the bands, but with a different order of magnitude of these widths. These differences are due to the fact that in [19, Theorem 8.1], the potential is supposed to be analytic, which is not the case for us.

**2.5. Some open questions.** We address some open questions which naturally arose in our research on the periodic Airy-Schrödinger operator.

- (1) A first question is to generalize our results for a potential which is no longer our explicit potential. We consider a function  $V$  which is analytic, such that  $V(0) = 0$  and  $V'(0) \neq 0$  and then we consider the  $2L_0$ -periodic function  $W$  defined on  $[-L_0, L_0]$  by:

$$\forall x \in [-L_0, L_0], W(x) = V(|x|).$$

Using perturbation theory techniques like those developed in [3] or [4], one would like to obtain similar results as Theorem 1, 3, 6 or 7.

- (2) Another question is to look at our model no longer on the real line but on the space  $\mathbb{R}^d$  for  $d \geq 1$ . A first result was obtained in the very simple case of  $H_d$  introduced in (11), but one hopes to use our results on the spectrum of  $H$  to study other periodic operators at least in dimension 2. In this case, we could be able to tackle the case where our operator decompose into a tensor product of two periodic Airy-Schrödinger operators with eventually two different characteristic lengths  $L_0$  and  $L_1$ . In this case the spectrum of the two-dimensional operator is the superposition of the band spectra of the

two one-dimensional operators. It would certainly lead to difficulties linked to the compared arithmetic natures of  $L_0$  and  $L_1$ , like those presented in [10].

- (3) Another interesting generalization would be to obtain asymptotic results like Theorem 6 or Theorem 7 for our non-analytic potential, in all the regimes considered in [19].
- (4) One last open question is the one of the eventual meromorphic continuation of the resolvent of the periodic Airy-Schrödinger operator to the spectral bands, using techniques like those in [11, 23]. It would lead to the question of the existence and the description of the resonances for the periodic Airy-Schrödinger operator.

**2.6. Outline of the paper.** In Section 3, we recall the classical theory of periodic operators and their band spectra. It allows us to get the equations to be solved to determine the edges of the spectral bands. In Section 4, we study the asymptotics of the canonical solutions, their derivatives and the asymptotics of their zeroes. These very precise asymptotics imply an important result of separation and ordering of the zeroes of the canonical solutions and their derivatives (Corollary 3). This result is the key result which allows to distinguish the upper edge of a spectral band from the lower edge of the next spectral band among the solutions of the equations obtained in Section 3. This identification of the spectral edges is performed in Sections 6 and 7.

The Section 5 is devoted to the study of families of strictly monotonous and continuous functions which allows to prove in Sections 6 and 7 the existence of solutions to the equations which define the spectral edges. Section 5 describes also the graphical interpretation of these equations, in terms of the functions  $\frac{v}{u}$  and  $\frac{v'}{u'}$ , which has guided our analysis throughout this paper.

Section 6.2 is devoted to the proof of Theorem 3. This proof contains most of the ideas used later in Section 4 to get all the asymptotics of the width of the spectral bands and of the spectral gaps in the semiclassical limit. We also investigate in Section 6.3 the behaviour of the upper edge of the first spectral band in both semiclassical and classical limits. In the classical limit, the integer  $p_0$  introduced in (7) plays a crucial role. In Section 7 we characterize the spectral edges of all the spectral bands in the range of  $V$ , we count these bands and we prove Theorem 4. We also prove the result on the spectral density in the range of  $V$ .

In Appendix B, the monotonicity of the functions  $z_k$  introduced in Lemma 4 is proven. This monotonicity result is particularly technical and requires a version of the Sturm Picone's lemma about interlacing of zeroes of solutions of ordinary differential equations adapted to our setting ([6]). Such result is proven in Appendix A.

### 3. THE BAND STRUCTURE OF THE SPECTRUM OF $H$

In this section we recall the equations characterizing the spectral edges of the spectrum of the operator  $H$ , using the general theory of periodic Schrödinger operators ([26]). Let  $\omega \in [-L_0, L_0]$ . We start by considering 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

$$\forall x \in \mathbb{R}, \psi(x + 2L_0) = e^{i(\frac{\pi}{L_0}\omega + \pi)}\psi(x). \quad (20)$$

Note that, as  $H^2([-L_0, L_0]) \subset C^1([-L_0, L_0])$ , this condition is equivalent to the boundary conditions:

$$\psi(L_0) = e^{i(\frac{\pi}{L_0}\omega + \pi)}\psi(-L_0) \quad \text{and} \quad \psi'(L_0) = e^{i(\frac{\pi}{L_0}\omega + \pi)}\psi'(-L_0). \quad (21)$$

The operator  $H(\omega)$  is self-adjoint. It is Hilbert-Schmidt and thus compact. Its spectrum is pure point and the eigenvalues of  $H(\omega)$  are solutions of explicit equations. According to [26],  $H$  is the direct integral of the operators  $H(\omega)$ :

$$H = \int_{[-L_0, L_0]}^{\oplus} H(\omega) d\omega.$$

This decomposition in direct integral allows to recover the spectrum of  $H$  from the spectra of the  $H(\omega)$ 's.

From the canonical solutions  $u$  and  $v$  of the Airy equation, one defines the canonical pair of odd and even solutions of (2) on the interval  $[-L_0, L_0]$ . These functions, denoted by  $U_\theta$  and  $V_\theta$  are defined, for every  $x \in [-L_0, L_0]$ , by

$$U_\theta(x) = -v'(-\theta V_0 - \theta E)u(\theta(V(x) - E)) + u'(-\theta V_0 - \theta E)v(\theta(V(x) - E))$$

and

$$V_\theta(x) = \text{sign}(x) (-v(-\theta V_0 - \theta E)u(\theta(V(x) - E)) + u(-\theta V_0 - \theta E)v(\theta(V(x) - E))).$$

They form a basis of even and odd  $C^1$  solutions of the equation (2) on the interval  $[-L_0, L_0]$ . Their wronskian satisfies

$$\forall x \in [L_0, L_0], (U_\theta V'_\theta - U'_\theta V_\theta)(x) = 1.$$

Since any solution of (2) is a linear combination of  $U_\theta$  and  $V_\theta$ , the boundary conditions (21) rewrite:

$$AU_\theta(L_0) + BV_\theta(L_0) = -e^{i(\frac{\pi}{L_0}\omega)} (AU_\theta(L_0) - BV_\theta(L_0)) \quad (22)$$

$$AU'_\theta(L_0) + BV'_\theta(L_0) = -e^{i(\frac{\pi}{L_0}\omega)} (-AU'_\theta(L_0) + BV'_\theta(L_0)), \quad (23)$$

for  $A, B \in \mathbb{R}$ . Thus,  $A$  and  $B$  are solution of the linear system:

$$\begin{cases} U_\theta(L_0) \left(1 + e^{i(\frac{\pi}{L_0}\omega)}\right) A + V_\theta(L_0) \left(1 - e^{i(\frac{\pi}{L_0}\omega)}\right) B = 0 \\ U'_\theta(L_0) \left(1 - e^{i(\frac{\pi}{L_0}\omega)}\right) A + V'_\theta(L_0) \left(1 + e^{i(\frac{\pi}{L_0}\omega)}\right) B = 0 \end{cases}. \quad (24)$$

Considering the system (24), one gets that  $E \in \mathbb{R}$  is an eigenvalue of  $H(\omega)$  if and only if

$$\begin{vmatrix} U_\theta(L_0)(1 + e^{i(\frac{\pi}{L_0}\omega)}) & V_\theta(L_0)(1 - e^{i(\frac{\pi}{L_0}\omega)}) \\ U'_\theta(L_0)(1 - e^{i(\frac{\pi}{L_0}\omega)}) & V'_\theta(L_0)(1 + e^{i(\frac{\pi}{L_0}\omega)}) \end{vmatrix} = 0. \quad (25)$$

The determinant in (25) being analytic in  $E$ , equation (25) has only a discrete set of solutions in  $E$  (since this determinant is not equal to 0 for every  $E$ ) which is consistent with the fact that  $H(\omega)$  is a compact operator. For  $\omega = -L_0$ , we get that (25) is equivalent to

$$-4U'_\theta(L_0) \cdot V_\theta(L_0) = 0. \quad (26)$$

For  $\omega = 0$ , we get that (25) is equivalent to

$$4U_\theta(L_0) \cdot V'_\theta(L_0) = 0. \quad (27)$$

Since the expression in the left member of (26) is analytic in  $E$  we can denote by  $E_{\min}^0 \leq E_{\max}^1 \leq E_{\min}^2 \leq E_{\max}^3 \leq \dots$  the elements of the spectrum of  $H(-L_0)$ ,

$$\sigma(H(-L_0)) := \{E_{\min}^0, E_{\max}^1, E_{\min}^2, E_{\max}^3, \dots\} = \left\{ E \in \mathbb{R}, U_{\theta}'(L_0) \cdot V_{\theta}(L_0) = 0 \right\}$$

and we denote by  $E_{\max}^0 \leq E_{\min}^1 \leq E_{\max}^2 \leq E_{\min}^3 \leq \dots$  the elements of the spectrum of  $H(0)$

$$\sigma(H(0)) := \{E_{\max}^0, E_{\min}^1, E_{\max}^2, E_{\min}^3, \dots\} = \left\{ E \in \mathbb{R}, U_{\theta}(L_0) \cdot V_{\theta}'(L_0) = 0 \right\}.$$

Then, using [26, Theorem XIII.90], we finally get the description of the spectrum of  $H$  as a band spectrum:

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

Moreover  $\sigma(H)$  is purely absolutely continuous and  $H$  has no eigenvalues. To compute the spectrum of  $H$ , it remains to determine the edges of the spectral bands  $E_{\min}^p$  and  $E_{\max}^p$  for  $p \geq 0$ .

**Remark.** Recall that the result here applies for any periodic potential and thus our computations and the description of the spectrum as a band spectrum are valid for any symmetric potential.

#### 4. ASYMPTOTICS OF THE CANONICAL SOLUTIONS AND OF THEIR ZEROES

The aim of this Section is to obtain precise estimates of the roots of  $u, v, u'$  and  $v'$ . This will be a consequence of the asymptotic expansions of the canonical solutions of the Airy equation on  $\mathbb{R}_-$ .

**4.1. Asymptotics of the canonical solutions.** In order to obtain asymptotic expansions of the canonical solutions of the Airy equation, we start with asymptotic expansions of the Airy functions  $Ai, Bi$  and their derivatives which are deduced from Bessel functions for which asymptotic expansions are well known.

For this purpose, one defines functions  $P(\nu, \cdot)$  and  $Q(\nu, \cdot)$  for any real number  $\nu$  through the Bessel functions  $J_{\nu}$  and  $Y_{\nu}$  (see [21])

$$P(\nu, \xi) = \sqrt{\frac{\pi\xi}{2}} \left( J_{\nu}(\xi) \cos \left( \xi - \frac{1}{2}\nu\pi - \frac{1}{4}\pi \right) + Y_{\nu}(\xi) \sin \left( \xi - \frac{1}{2}\nu\pi - \frac{1}{4}\pi \right) \right)$$

and

$$Q(\nu, \xi) = \sqrt{\frac{\pi\xi}{2}} \left( Y_{\nu}(\xi) \cos \left( \xi - \frac{1}{2}\nu\pi - \frac{1}{4}\pi \right) - J_{\nu}(\xi) \sin \left( \xi - \frac{1}{2}\nu\pi - \frac{1}{4}\pi \right) \right).$$

The functions  $P(\nu, \cdot)$  and  $Q(\nu, \cdot)$  have known expansions which are used to get asymptotic expansions of the canonical solutions and their derivatives. Note that, when  $\xi$  tends to  $+\infty$ ,  $P(\nu, \xi) \sim 1$  and  $Q(\nu, \xi) \sim \frac{4\nu^2-1}{8\xi}$ .

**Proposition 2.** *For every  $x > 0$ , we set  $\xi = \frac{2}{3}x^{\frac{3}{2}}$ . We have:*

$$u(-x) = 2\pi^{\frac{1}{2}}x^{-\frac{1}{4}}Ai'(0) \left( \sin\left(\xi - \frac{7\pi}{12}\right) P\left(\frac{1}{3}, \xi\right) + \cos\left(\xi - \frac{7\pi}{12}\right) Q\left(\frac{1}{3}, \xi\right) \right), \quad (28)$$

$$u'(-x) = -2\pi^{\frac{1}{2}}x^{\frac{1}{4}}Ai'(0) \left( \cos\left(\xi - \frac{7\pi}{12}\right) P\left(\frac{2}{3}, \xi\right) - \sin\left(\xi - \frac{7\pi}{12}\right) Q\left(\frac{2}{3}, \xi\right) \right), \quad (29)$$

$$v(-x) = -2\pi^{\frac{1}{2}}x^{-\frac{1}{4}}Ai(0) \left( \sin\left(\xi + \frac{\pi}{12}\right) P\left(\frac{1}{3}, \xi\right) + \cos\left(\xi + \frac{\pi}{12}\right) Q\left(\frac{1}{3}, \xi\right) \right), \quad (30)$$

$$v'(-x) = -2\pi^{\frac{1}{2}}x^{\frac{1}{4}}Ai(0) \left( -\cos\left(\xi + \frac{\pi}{12}\right) P\left(\frac{2}{3}, \xi\right) + \sin\left(\xi + \frac{\pi}{12}\right) Q\left(\frac{2}{3}, \xi\right) \right). \quad (31)$$

Before proving Proposition 2 we need the following technical lemma.

**Lemma 1.** *For every  $\xi > \frac{1}{\sqrt{26}}$ ,  $P\left(\frac{1}{3}, \xi\right) > 0$  and we have*

$$\forall \xi > \frac{1}{\sqrt{13}}, \quad \left| \frac{Q\left(\frac{1}{3}, \xi\right)}{P\left(\frac{1}{3}, \xi\right)} \right| < \frac{5}{36\xi}. \quad (32)$$

*For every  $\xi > \frac{1}{\sqrt{22}}$ ,  $P\left(\frac{2}{3}, \xi\right) > 0$  and we have*

$$\forall \xi > \frac{1}{\sqrt{11}}, \quad \left| \frac{Q\left(\frac{2}{3}, \xi\right)}{P\left(\frac{2}{3}, \xi\right)} \right| < \frac{7}{12\xi}. \quad (33)$$

*Proof:* Using [1, 9.2.9 and 9.2.10], we have

$$\forall \xi > 0, \quad \left| P\left(\frac{1}{3}, \xi\right) - 1 \right| \leq \frac{5 \times 77}{81 \times 128 \times \xi^2} < \frac{1}{26\xi^2} \quad (34)$$

and

$$\forall \xi > 0, \quad \left| Q\left(\frac{1}{3}, \xi\right) + \frac{5}{72\xi} \right| \leq \frac{5 \times 77 \times 221}{6 \times 9^3 \times 8^3 \times \xi^3} < \frac{1}{26\xi^3}. \quad (35)$$

In particular, we deduce from (34) that for every  $\xi > \frac{1}{\sqrt{26}}$ ,  $P\left(\frac{1}{3}, \xi\right) > 0$ . Then, (34) and (35) imply

$$\forall \xi > \frac{1}{\sqrt{13}}, \quad \left| \frac{Q\left(\frac{1}{3}, \xi\right)}{P\left(\frac{1}{3}, \xi\right)} \right| < \frac{\frac{5}{72\xi} - \frac{1}{26\xi^3}}{1 - \frac{1}{26\xi^2}} < \frac{5}{36\xi},$$

which proves (32). Indeed, for  $\xi > \frac{1}{\sqrt{13}}$ ,  $\frac{1}{1 - \frac{1}{26\xi^2}} < 2$ .

Using again [1, 9.2.9 and 9.2.10], we also have

$$\forall \xi > 0, \quad \left| P\left(\frac{2}{3}, \xi\right) - 1 \right| \leq \frac{7 \times 65}{81 \times 128 \times \xi^2} < \frac{1}{22\xi^2} \quad (36)$$

and

$$\forall \xi > 0, \quad \left| Q\left(\frac{2}{3}, \xi\right) - \frac{7}{72\xi} \right| \leq \frac{7 \times 65 \times 209}{6 \times 9^3 \times 8^3 \times \xi^3} < \frac{1}{22\xi^3}. \quad (37)$$

In particular, for every  $\xi > \frac{1}{\sqrt{22}}$ ,  $P\left(\frac{2}{3}, \xi\right) > 0$ . Then, (36) and (37) imply

$$\forall \xi > \frac{1}{\sqrt{11}}, \quad \left| \frac{Q\left(\frac{2}{3}, \xi\right)}{P\left(\frac{2}{3}, \xi\right)} \right| < \frac{\frac{7}{72\xi} + \frac{1}{22\xi^3}}{1 - \frac{1}{22\xi^2}} < \frac{7}{36\xi} + \frac{1}{11\xi^3} < \frac{7}{12\xi},$$

which proves (33). Indeed, for  $\xi > \frac{1}{\sqrt{11}}$ ,  $\frac{1}{1 - \frac{1}{22\xi^2}} < 2$  and  $\frac{7}{36\xi} + \frac{1}{11\xi^3} < \frac{7}{12\xi}$ .  $\square$

With (28), (34) and (35), we get

$$u(-a_{j+1}) = 2\pi^{\frac{1}{2}}(a_{j+1})^{-\frac{1}{4}}Ai'(0) + \mathcal{O}\left((a_{j+1})^{-\frac{3}{2}}\right)$$

which implies (18). Similarly, with (29), (36) and (37), we get

$$u'(-\tilde{a}_{j+1}) = 2\pi^{\frac{1}{2}}(\tilde{a}_{j+1})^{\frac{1}{4}}Ai'(0) + \mathcal{O}\left((\tilde{a}_{j+1})^{-\frac{3}{2}}\right)$$

which implies (18).

We turn to the proof of Proposition 2.

*Proof:* Let  $x > 0$  and  $\xi = \frac{2}{3}x^{\frac{3}{2}}$ . The functions  $Ai$ ,  $Bi$  and their derivatives are related to the Bessel functions through the relations (see [1, 10.4.15 and after])

$$Ai(-x) = \frac{1}{3}\sqrt{x}\left(J_{\frac{1}{3}}(\xi) + J_{-\frac{1}{3}}(\xi)\right), \quad Bi(-x) = \sqrt{\frac{x}{3}}\left(J_{-\frac{1}{3}}(\xi) - J_{\frac{1}{3}}(\xi)\right)$$

and

$$Ai'(-x) = -\frac{1}{3}x\left(J_{-\frac{2}{3}}(\xi) - J_{\frac{2}{3}}(\xi)\right), \quad Bi'(-x) = \frac{x}{\sqrt{3}}\left(J_{-\frac{2}{3}}(\xi) + J_{\frac{2}{3}}(\xi)\right).$$

Thus, we have the following expressions for the Airy functions and their derivatives on the negative half-line:

$$Ai(-x) = \pi^{-\frac{1}{2}}x^{-\frac{1}{4}}\left(\cos\left(\xi - \frac{\pi}{4}\right)P\left(\frac{1}{3}, \xi\right) - \sin\left(\xi - \frac{\pi}{4}\right)Q\left(\frac{1}{3}, \xi\right)\right), \quad (38)$$

$$Ai'(-x) = \pi^{-\frac{1}{2}}x^{\frac{1}{4}}\left(\sin\left(\xi - \frac{\pi}{4}\right)P\left(\frac{2}{3}, \xi\right) + \cos\left(\xi - \frac{\pi}{4}\right)Q\left(\frac{2}{3}, \xi\right)\right), \quad (39)$$

$$Bi(-x) = -\pi^{-\frac{1}{2}}x^{-\frac{1}{4}}\left(\sin\left(\xi - \frac{\pi}{4}\right)P\left(\frac{1}{3}, \xi\right) + \cos\left(\xi - \frac{\pi}{4}\right)Q\left(\frac{1}{3}, \xi\right)\right), \quad (40)$$

$$Bi'(-x) = \pi^{-\frac{1}{2}}x^{\frac{1}{4}}\left(\cos\left(\xi - \frac{\pi}{4}\right)P\left(\frac{2}{3}, \xi\right) - \sin\left(\xi - \frac{\pi}{4}\right)Q\left(\frac{2}{3}, \xi\right)\right). \quad (41)$$

Before getting similar expressions for the canonical solutions  $u$  and  $v$ , let us start by rewriting  $u$  and  $v$ , observing that  $\frac{Bi'(0)}{Ai'(0)} = -\sqrt{3} = -\tan\left(\frac{\pi}{3}\right)$ :

$$\begin{aligned} \forall x \in \mathbb{R}, u(x) &= \pi(Bi'(0)Ai(x) - Ai'(0)Bi(x)) \\ &= -2\pi Ai'(0)\left(\cos\left(\frac{\pi}{3}\right)Bi(x) + \sin\left(\frac{\pi}{3}\right)Ai(x)\right). \end{aligned} \quad (42)$$

Similarly,

$$\forall x \in \mathbb{R}, v(x) = 2\pi Ai(0)\left(\cos\left(\frac{\pi}{3}\right)Bi(x) - \sin\left(\frac{\pi}{3}\right)Ai(x)\right). \quad (43)$$

Combining (42), (38) and (40) one gets, for every  $x > 0$ ,

$$\begin{aligned} u(-x) &= -2\pi Ai'(0)\left(\cos\left(\frac{\pi}{3}\right)Bi(-x) + \sin\left(\frac{\pi}{3}\right)Ai(-x)\right) \\ &= -2\pi^{\frac{1}{2}}x^{-\frac{1}{4}}Ai'(0)\left(\left(-\cos\left(\frac{\pi}{3}\right)\sin\left(\xi - \frac{\pi}{4}\right) + \sin\left(\frac{\pi}{3}\right)\cos\left(\xi - \frac{\pi}{4}\right)\right)P\left(\frac{1}{3}, \xi\right) + \right. \\ &\quad \left. \left(-\cos\left(\frac{\pi}{3}\right)\cos\left(\xi - \frac{\pi}{4}\right) - \sin\left(\frac{\pi}{3}\right)\sin\left(\xi - \frac{\pi}{4}\right)\right)Q\left(\frac{1}{3}, \xi\right)\right) \\ &= -2\pi^{\frac{1}{2}}x^{-\frac{1}{4}}Ai'(0)\left(\sin\left(-\xi + \frac{\pi}{4} + \frac{\pi}{3}\right)P\left(\frac{1}{3}, \xi\right) - \cos\left(-\xi + \frac{\pi}{4} + \frac{\pi}{3}\right)Q\left(\frac{1}{3}, \xi\right)\right) \\ &= 2\pi^{\frac{1}{2}}x^{-\frac{1}{4}}Ai'(0)\left(\sin\left(\xi - \frac{7\pi}{12}\right)P\left(\frac{1}{3}, \xi\right) + \cos\left(\xi - \frac{7\pi}{12}\right)Q\left(\frac{1}{3}, \xi\right)\right). \end{aligned}$$

By derivating (42) and doing similar computations as in (28) one gets:

$$\forall x > 0, u'(-x) = -2\pi^{\frac{1}{2}}x^{\frac{1}{4}}Ai'(0)\left(\cos\left(\xi - \frac{7\pi}{12}\right)P\left(\frac{2}{3}, \xi\right) - \sin\left(\xi - \frac{7\pi}{12}\right)Q\left(\frac{2}{3}, \xi\right)\right).$$

The expressions for  $v$  and  $v'$  are obtained the same way.  $\square$



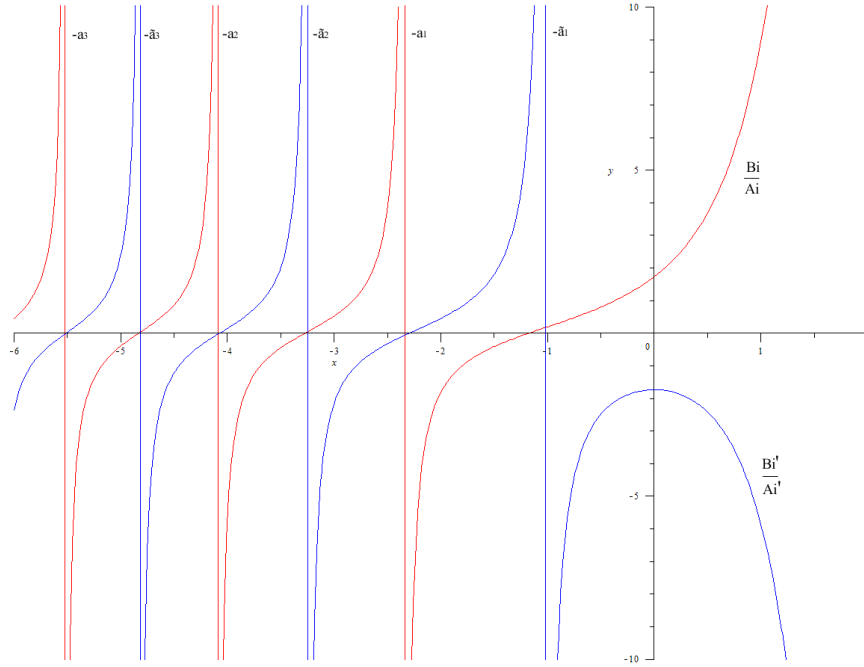
**Remark.** Note that  $x \mapsto \pi^{-\frac{1}{2}}x^{-\frac{1}{4}}\cos(\xi - \frac{\pi}{4})$  and  $x \mapsto \pi^{-\frac{1}{2}}x^{-\frac{1}{4}}\sin(\xi - \frac{\pi}{4})$  are solutions of the equation  $y'' = (-x + \frac{5}{16x^2})y$  and thus are approximate solutions of  $y'' = -xy$ . Hence the existence of  $P$  and  $Q$  can be seen as an application of the Duhamel principle.

#### 4.2. Asymptotics and ordering of the zeroes of the canonical solutions.

Before having precise intervals in which we can localize the zeroes of  $u, u', v$  and  $v'$ , we localize them between zeroes of the classical Airy function  $Ai$  and its derivative. Since the zeroes of  $Ai$  and  $Ai'$  are known, it will guide us to choose the good intervals in which we will verify that  $u, u', v$  and  $v'$  do vanish and outside of which they do not.

We start by looking at the variations of the functions  $\frac{Bi}{Ai}$  and  $\frac{Bi'}{Ai'}$ . The functions  $\frac{Bi}{Ai}$  and  $\frac{Bi'}{Ai'}$  have the following behaviours:

- On every interval  $(-a_{j+1}, -a_j)$ , the function  $\frac{Bi}{Ai}$  is continuous, increasing and is a bijection from  $(-a_{j+1}, -a_j)$  to  $\mathbb{R}$ . Moreover,  $\frac{Bi'}{Ai'}$  is continuous, increasing and is a bijection from  $(-a_1, +\infty)$  to  $\mathbb{R}$ .
- On every interval  $(-\tilde{a}_{j+1}, -\tilde{a}_j)$ , the function  $\frac{Bi'}{Ai'}$  is continuous, increasing and is a bijection from  $(-\tilde{a}_{j+1}, -\tilde{a}_j)$  to  $\mathbb{R}$ . Moreover,  $\frac{Bi}{Ai}$  is continuous and increasing on  $(-\tilde{a}_1, 0]$  from  $-\infty$  to 0. It is also continuous, decreasing and a bijection from  $(-\infty, 0]$  to  $[0, +\infty)$ .



Note that the roots of  $u$ ,  $v$ ,  $u'$  and  $v'$  are exactly the solutions of the equations  $\frac{Bi}{Ai}(x) = \frac{Bi'}{Ai'}(0)$ ,  $\frac{Bi}{Ai}(x) = \frac{Bi}{Ai}(0)$ ,  $\frac{Bi'}{Ai'}(x) = \frac{Bi'}{Ai'}(0)$  and  $\frac{Bi'}{Ai'}(x) = \frac{Bi}{Ai}(0)$ , respectively. We will identify the solutions of these equations and the sequences of zeroes introduced in Section 1.

The equation in  $x$

$$\frac{Bi}{Ai}(x) = \frac{Bi'}{Ai'}(0) = -\sqrt{3}$$

has a countable number of solutions which are negative and no positive solution. Let us denote by  $(-\tilde{c}_{2j})_{j \geq 0}$  the sequence of all the solutions arranged in decreasing order with, for every  $j \geq 0$ ,  $-\tilde{c}_{2j} \in (-a_{j+1}, -\tilde{a}_{j+1})$ . Since the sets of the zeroes of  $Ai$  and of  $u$  are disjoint, **the set of the zeroes of  $u$  is exactly**  $\{-\tilde{c}_{2j}\}_{j \geq 0}$ .

Similarly, the equation in  $x$

$$\frac{Bi'}{Ai'}(x) = \frac{Bi'}{Ai'}(0) = -\sqrt{3}$$

has a countable number of solutions which are negative and no positive solution except 0. Let us denote by  $(-\tilde{c}_{2j+1})_{j \geq 0}$  the sequence of all the solutions arranged in decreasing order with, for every  $j \geq 0$ ,  $-\tilde{c}_{2j+1} \in (-\tilde{a}_{j+2}, -a_{j+1})$ . Since the sets of the zeroes of  $Ai'$  and of  $u'$  are disjoint, **the set of the zeroes of  $u'$  is exactly**  $\{-\tilde{c}_{2j+1}\}_{j \geq 0} \cup \{0\}$ .

The equation in  $x$

$$\frac{Bi}{Ai}(x) = \frac{Bi}{Ai}(0) = \sqrt{3}$$

has a countable number of solutions which are negative and no positive solution except 0. Let us denote by  $(-c_{2j+1})_{j \geq 0}$  the sequence of all the solutions arranged in decreasing order with, for every  $j \geq 0$ ,  $-c_{2j+1} \in (-\tilde{a}_{j+2}, -a_{j+1})$ . Since the sets of the zeroes of  $Ai$  and of  $v$  are disjoint, **the set of the zeroes of  $v$  is exactly**  $\{-c_{2j+1}\}_{j \geq 0} \cup \{0\}$ .

Finally, the equation in  $x$

$$\frac{Bi'}{Ai'}(x) = \frac{Bi}{Ai}(0) = \sqrt{3}$$

also has a countable number of solutions which are negative and no positive solution. Let us denote by  $(-c_{2j})_{j \geq 0}$  the sequence of all the solutions arranged in decreasing order with, for every  $j \geq 0$ ,  $-c_{2j} \in (-a_{j+1}, -\tilde{a}_{j+1})$ . Since the sets of the zeroes of  $Ai'$  and of  $v'$  are disjoint, **the set of the zeroes of  $v'$  is exactly**  $\{-c_{2j}\}_{j \geq 0}$ .

From the asymptotic expansions (28), (29), (30) and (31) and the distribution of the sequences of zeroes of  $Ai$  and  $Ai'$ , we can get intervals in which we localize the constants  $-c_k$  and  $-\tilde{c}_k$ . We also obtain the variations of  $u$  and  $v$ .

**Proposition 3.** (1) *For every  $j \geq 0$ , the function  $v'$  has a unique zero in the interval  $(-\left(\frac{3}{2}(j\pi + \frac{\pi}{2})\right)^{\frac{2}{3}}, -\left(\frac{3}{2}(j\pi + \frac{\pi}{3})\right)^{\frac{2}{3}})$  and does not vanish outside of these intervals. Thus,*

$$-c_{2j} \in \left(-\left(\frac{3}{2}(j\pi + \frac{\pi}{2})\right)^{\frac{2}{3}}, -\left(\frac{3}{2}(j\pi + \frac{\pi}{3})\right)^{\frac{2}{3}}\right). \quad (44)$$

(2) *For every  $j \geq 0$ , the function  $u$  has a unique zero in the interval*

$(-\left(\frac{3}{2}(j\pi + \frac{2\pi}{3})\right)^{\frac{2}{3}}, -\left(\frac{3}{2}(j\pi + \frac{\pi}{2})\right)^{\frac{2}{3}})$  and does not vanish outside of these intervals. Thus,

$$-\tilde{c}_{2j} \in \left(-\left(\frac{3}{2}(j\pi + \frac{2\pi}{3})\right)^{\frac{2}{3}}, -\left(\frac{3}{2}(j\pi + \frac{\pi}{2})\right)^{\frac{2}{3}}\right). \quad (45)$$

(3) For every  $j \geq 0$ , the function  $v$  has a unique zero in the interval

$(-\left(\frac{3}{2}(j\pi + \pi)\right)^{\frac{2}{3}}, -\left(\frac{3}{2}(j\pi + \frac{5\pi}{6})\right)^{\frac{2}{3}})$  and does not vanish outside of these intervals. Thus,

$$-c_{2j+1} \in \left(-\left(\frac{3}{2}(j\pi + \pi)\right)^{\frac{2}{3}}, -\left(\frac{3}{2}(j\pi + \frac{5\pi}{6})\right)^{\frac{2}{3}}\right). \quad (46)$$

(4) For every  $j \geq 0$ , the function  $u'$  has a unique zero in the interval

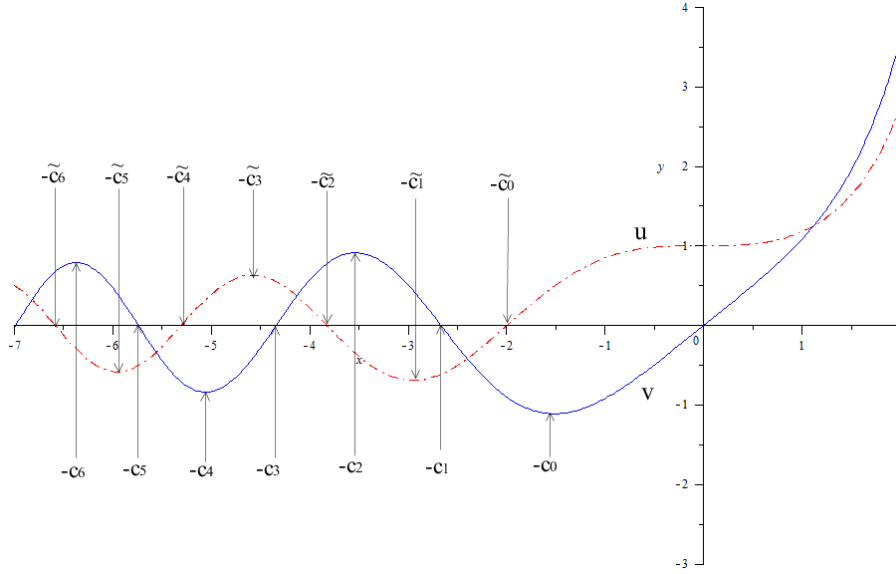
$(-\left(\frac{3}{2}(j\pi + \frac{7\pi}{6})\right)^{\frac{2}{3}}, -\left(\frac{3}{2}(j\pi + \pi)\right)^{\frac{2}{3}})$  and does not vanish outside of these intervals. Thus,

$$-\tilde{c}_{2j+1} \in \left(-\left(\frac{3}{2}(j\pi + \frac{7\pi}{6})\right)^{\frac{2}{3}}, -\left(\frac{3}{2}(j\pi + \pi)\right)^{\frac{2}{3}}\right). \quad (47)$$

**Proposition 4.** *The variations of  $u$  and  $v$  and their signs between two consecutive zeroes are:*

- $u$  is positive on  $(-\tilde{c}_0, +\infty)$  and for every  $j \geq 0$ ,  $(-1)^j u$  is negative on  $[-\tilde{c}_{2j+2}, -\tilde{c}_{2j}]$ . It is strictly increasing on  $(-\tilde{c}_1, +\infty)$ , and for every  $j \geq 0$ ,  $(-1)^j u$  is strictly decreasing on  $[-\tilde{c}_{2j+3}, -\tilde{c}_{2j+1}]$ .
- $v$  is positive on  $[0, +\infty)$ , negative on  $[-c_1, 0]$  and for every  $j \geq 0$ ,  $(-1)^j v$  is positive on  $[-c_{2j+3}, -c_{2j+1}]$ . It is strictly increasing on  $(-c_0, +\infty)$ , and for every  $j \geq 0$ ,  $(-1)^j v$  is strictly decreasing on  $[-c_{2j+2}, -c_{2j}]$ .

The respective behaviour of  $u$  and  $v$  on respectively the intervals  $(-\tilde{c}_0, +\infty)$  and  $(-c_1, +\infty)$  are different than their respective behaviour on respectively the intervals  $(-\infty, -\tilde{c}_0]$  and  $(-\infty, -c_1]$ .



We prove simultaneously Proposition 3 and Proposition 4.

*Proof:* Before starting the proof, since  $-(\frac{\pi}{2})^{\frac{2}{3}} > -\tilde{a}_1 > -c_0$ , we stress that  $v'$  does not vanish in the interval  $(-(\frac{\pi}{2})^{\frac{2}{3}}, +\infty)$  which justifies the starting point for the numbering of the  $-c_{2j}$ . Similarly, the only root of  $v$  in the interval  $(-(\frac{5\pi}{4})^{\frac{2}{3}}, +\infty)$  is 0, which justifies the numbering of the  $-c_{2j+1}$ ,  $u$  does not vanish in  $(-(\frac{3\pi}{4})^{\frac{2}{3}}, +\infty)$  and the only root of  $u'$  in the interval  $(-(\frac{3\pi}{2})^{\frac{2}{3}}, +\infty)$  is 0, which justifies the numbering of respectively the  $-\tilde{c}_{2j}$  and the  $-\tilde{c}_{2j+1}$ .

We prove only the assertion on  $u$  and  $-\tilde{c}_{2j}$ , the others are proved in a completely similar way. We use the following method: thanks to the knowledge of  $\frac{Q}{P}$  for  $\xi > \frac{1}{\sqrt{11}}$ , we are able to show that  $u$  changes its sign at the two boundary values of the considered interval while  $u'$  is of constant sign in the interval.

Let  $j \geq 0$ . Using (28) for  $x = (\frac{3}{2}(j\pi + \frac{2\pi}{3}))^{\frac{2}{3}}$  and thus  $\xi = j\pi + \frac{2\pi}{3}$ , one gets:

$$u\left(-\left(\frac{3}{2}(j\pi + \frac{2\pi}{3})\right)^{\frac{2}{3}}\right) = 2\pi^{\frac{1}{2}} \left(\frac{3}{2}(j\pi + \frac{2\pi}{3})\right)^{-\frac{1}{6}} Ai'(0)(-1)^j \sin\left(\frac{\pi}{12}\right) \times \\ P\left(\frac{1}{3}, j\pi + \frac{2\pi}{3}\right) \left(1 + \cotan\left(\frac{\pi}{12}\right) \frac{Q\left(\frac{1}{3}, j\pi + \frac{2\pi}{3}\right)}{P\left(\frac{1}{3}, j\pi + \frac{2\pi}{3}\right)}\right).$$

But,  $\cotan\left(\frac{\pi}{12}\right) = 2 + \sqrt{3}$  and since using (32),

$$\left|\cotan\left(\frac{\pi}{12}\right) \frac{Q\left(\frac{1}{3}, j\pi + \frac{2\pi}{3}\right)}{P\left(\frac{1}{3}, j\pi + \frac{2\pi}{3}\right)}\right| < \frac{5(2 + \sqrt{3})}{36} < \frac{2}{3},$$

we get that

$$\left(1 + \cotan\left(\frac{\pi}{12}\right) \frac{Q\left(\frac{1}{3}, j\pi + \frac{2\pi}{3}\right)}{P\left(\frac{1}{3}, j\pi + \frac{2\pi}{3}\right)}\right) > 0.$$

Since  $\sin\left(\frac{\pi}{12}\right) > 0$ ,  $P\left(\frac{1}{3}, j\pi + \frac{2\pi}{3}\right) > 0$  and  $Ai'(0) < 0$ ,

$$(-1)^j u\left(-\left(\frac{3}{2}(2j\pi + \frac{9\pi}{12})\right)^{\frac{2}{3}}\right) < 0.$$

Then, using (28) for  $x = (\frac{3}{2}(j\pi + \frac{\pi}{3}))^{\frac{2}{3}}$  and thus  $\xi = j\pi + \frac{\pi}{3}$ , one gets:

$$u\left(-\left(\frac{3}{2}(j\pi + \frac{\pi}{3})\right)^{\frac{2}{3}}\right) = 2\pi^{\frac{1}{2}} \left(\frac{3}{2}(j\pi + \frac{\pi}{3})\right)^{-\frac{1}{6}} Ai'(0)(-1)^j \sin\left(-\frac{\pi}{12}\right) \times \\ P\left(\frac{1}{3}, j\pi + \frac{\pi}{3}\right) \left(1 + \cotan\left(-\frac{\pi}{12}\right) \frac{Q\left(\frac{1}{3}, j\pi + \frac{\pi}{3}\right)}{P\left(\frac{1}{3}, j\pi + \frac{\pi}{3}\right)}\right).$$

But, using (32),

$$\left|\cotan\left(-\frac{\pi}{12}\right) \frac{Q\left(\frac{1}{3}, j\pi + \frac{\pi}{3}\right)}{P\left(\frac{1}{3}, j\pi + \frac{\pi}{3}\right)}\right| < \frac{5(2 + \sqrt{3})}{36} < \frac{2}{3},$$

and we get that

$$\left(1 + \cotan\left(-\frac{\pi}{12}\right) \frac{Q\left(\frac{1}{3}, j\pi + \frac{\pi}{3}\right)}{P\left(\frac{1}{3}, j\pi + \frac{\pi}{3}\right)}\right) < 0.$$

Since  $P\left(\frac{1}{3}, j\pi + \frac{\pi}{3}\right) > 0$ ,

$$(-1)^j u\left(-\left(\frac{3}{2}(j\pi + \frac{\pi}{3})\right)^{\frac{2}{3}}\right) > 0.$$

If  $x \in [(\frac{3}{2}(j\pi + \frac{\pi}{3}))^{\frac{2}{3}}, (\frac{3}{2}(j\pi + \frac{2\pi}{3}))^{\frac{2}{3}}]$  then  $\xi - \frac{7\pi}{12} \in [j\pi - \frac{\pi}{12}, j\pi + \frac{\pi}{12}]$  and one has

$$\frac{\sqrt{2}}{2} \leq (-1)^j \cos\left(\xi - \frac{7\pi}{12}\right) \leq \frac{\sqrt{2+\sqrt{3}}}{2} \quad \text{and} \quad \frac{1}{2+\sqrt{3}} \leq \tan\left(\xi - \frac{7\pi}{12}\right) \leq 1.$$

Moreover, using (33) and  $\xi \geq \frac{\pi}{2}$ ,

$$\left| \frac{Q(\frac{2}{3}, \xi)}{P(\frac{2}{3}, \xi)} \right| < \frac{7}{12\xi} \leq \frac{14}{12\pi} < \frac{1}{2}.$$

Then, using (29), for every  $x \in [(\frac{3}{2}(j\pi + \frac{\pi}{3}))^{\frac{2}{3}}, (\frac{3}{2}(j\pi + \frac{2\pi}{3}))^{\frac{2}{3}}]$ ,

$$(-1)^j u'(-x) = 2\pi^{\frac{1}{2}} x^{\frac{1}{4}} Ai'(0) \cos\left(\xi - \frac{7\pi}{12}\right) P\left(\frac{2}{3}, \xi\right) \left(1 - \tan\left(\xi - \frac{7\pi}{12}\right) \frac{Q(\frac{2}{3}, \xi)}{P(\frac{2}{3}, \xi)}\right) > 0.$$

We deduce that  $u$  is continuous, strictly increasing for  $j$  even (respectively decreasing for  $j$  odd) from a negative value to a positive one (respectively from a positive value to a negative one) and thus has a unique zero in the interval  $[-(\frac{3}{2}(j\pi + \frac{2\pi}{3}))^{\frac{2}{3}}, -(\frac{3}{2}(j\pi + \frac{\pi}{3}))^{\frac{2}{3}}]$ , for every  $j \geq 0$ .

It remains to verify that  $u$  does not vanish on the interval

$$\left(-\left(\frac{3}{2}((j+1)\pi + \frac{\pi}{3})\right)^{\frac{2}{3}}, -\left(\frac{3}{2}(j\pi + \frac{2\pi}{3})\right)^{\frac{2}{3}}\right).$$

If  $x \in ((\frac{3}{2}(j\pi + \frac{2\pi}{3}))^{\frac{2}{3}}, (\frac{3}{2}((j+1)\pi + \frac{\pi}{3}))^{\frac{2}{3}})$  then  $\xi - \frac{7\pi}{12} \in [j\pi + \frac{\pi}{12}, j\pi + \frac{3\pi}{4}]$  and one has

$$\frac{1}{2\sqrt{2+\sqrt{3}}} \leq (-1)^j \sin\left(\xi - \frac{7\pi}{12}\right) \leq \frac{\sqrt{2}}{2} \quad \text{and} \quad 1 \leq \cotan\left(\xi - \frac{7\pi}{12}\right) \leq 2 + \sqrt{3}.$$

Moreover, using (33) and  $\xi \geq \frac{2\pi}{3}$ ,

$$\left| \cotan\left(\xi - \frac{7\pi}{12}\right) \frac{Q(\frac{1}{3}, \xi)}{P(\frac{1}{3}, \xi)} \right| < (2 + \sqrt{3}) \cdot \frac{7}{36\xi} < \frac{2}{3}$$

and using (29), for every  $x \in ((\frac{3}{2}(j\pi + \frac{2\pi}{3}))^{\frac{2}{3}}, (\frac{3}{2}((j+1)\pi + \frac{\pi}{3}))^{\frac{2}{3}})$ ,

$$(-1)^j u(-x) = 2\pi^{\frac{1}{2}} x^{-\frac{1}{4}} Ai'(0) (-1)^j \sin\left(\xi - \frac{7\pi}{12}\right) P\left(\frac{1}{3}, \xi\right) \left(1 + \cotan\left(\xi - \frac{7\pi}{12}\right) \frac{Q(\frac{1}{3}, \xi)}{P(\frac{1}{3}, \xi)}\right) < 0.$$

As  $-\tilde{c}_0 \in [-\pi^{\frac{2}{3}}, -(\frac{3\pi}{4})^{\frac{2}{3}}]$ , we deduce (45) by counting the constants  $-\tilde{c}_{2j}$  and the intervals in which  $u$  vanishes.  $\square$

From Proposition 3 we deduce immediately the ordering of the zeroes of the canonical solutions and their derivatives.

**Corollary 3.** *For every  $k \geq 0$ ,  $-\tilde{c}_k < -c_k$ .*

From Proposition 3, we also deduce asymptotics of the sequences  $(c_k)_{k \geq 0}$  and  $(\tilde{c}_k)_{k \geq 0}$ .

**Corollary 4.** *One has*

$$c_k = \left(\frac{3k\pi}{4}\right)^{\frac{2}{3}} + \mathcal{O}\left(\frac{1}{k^{\frac{1}{3}}}\right) \quad \text{and} \quad \tilde{c}_k - c_k = \left(\frac{\pi}{9\sqrt{2}}\right)^{\frac{2}{3}} \frac{1}{k^{\frac{1}{3}}} + \mathcal{O}\left(\frac{1}{k^{\frac{4}{3}}}\right). \quad (48)$$

*Proof:* The first estimate in (48) follows directly from the asymptotics proven in Lemma 2. For the difference between  $c_k$  and  $\tilde{c}_k$ , one uses (50)-(54) and (52)-(56). Indeed, for every  $j \geq 0$ ,

$$\tilde{c}_{2j} - c_{2j} = \left(\frac{3j\pi}{2}\right)^{\frac{2}{3}} \cdot \left(\frac{7}{18j} - \frac{5}{18j} + \mathcal{O}\left(\frac{1}{j^2}\right)\right) = \left(\frac{\pi}{18}\right)^{\frac{2}{3}} \frac{1}{j^{\frac{1}{3}}} + \mathcal{O}\left(\frac{1}{j^{\frac{4}{3}}}\right)$$

and similarly,

$$\tilde{c}_{2j+1} - c_{2j+1} = \left(\frac{\pi}{18}\right)^{\frac{2}{3}} \frac{1}{j^{\frac{1}{3}}} + \mathcal{O}\left(\frac{1}{j^{\frac{4}{3}}}\right),$$

which proves (48).  $\square$

We introduce, for every  $k \geq 0$ ,

$$\xi_k = \frac{2}{3}c_k^{\frac{3}{2}} \quad \text{and} \quad \tilde{\xi}_k = \frac{2}{3}\tilde{c}_k^{\frac{3}{2}}.$$

**Lemma 2.** *Let  $j \geq 0$ . One has*

$$\xi_{2j} \in \left[ \frac{5\pi}{12} + j\pi - \frac{7}{12(j\pi + \frac{\pi}{3})}, \frac{5\pi}{12} + j\pi + \frac{7}{12(j\pi + \frac{\pi}{3})} \right] \quad (49)$$

$$\text{and } c_{2j} = \left(\frac{3j\pi}{2}\right)^{\frac{2}{3}} \cdot \left(1 + \frac{5}{18j} + \mathcal{O}\left(\frac{1}{j^2}\right)\right), \quad (50)$$

$$\xi_{2j+1} \in \left[ \frac{11\pi}{12} + j\pi - \frac{5}{36(j\pi + \frac{5\pi}{6})}, \frac{11\pi}{12} + j\pi + \frac{5}{36(j\pi + \frac{5\pi}{6})} \right] \quad (51)$$

$$\text{and } c_{2j+1} = \left(\frac{3j\pi}{2}\right)^{\frac{2}{3}} \cdot \left(1 + \frac{11}{18j} + \mathcal{O}\left(\frac{1}{j^2}\right)\right), \quad (52)$$

$$\tilde{\xi}_{2j} \in \left[ \frac{7\pi}{12} + j\pi - \frac{5}{36(j\pi + \frac{\pi}{2})}, \frac{7\pi}{12} + j\pi + \frac{5}{36(j\pi + \frac{\pi}{2})} \right] \quad (53)$$

$$\text{and } \tilde{c}_{2j} = \left(\frac{3j\pi}{2}\right)^{\frac{2}{3}} \cdot \left(1 + \frac{7}{18j} + \mathcal{O}\left(\frac{1}{j^2}\right)\right), \quad (54)$$

$$\tilde{\xi}_{2j+1} \in \left[ \frac{13\pi}{12} + j\pi - \frac{7}{12(j+1)\pi}, \frac{13\pi}{12} + j\pi + \frac{7}{12(j+1)\pi} \right] \quad (55)$$

$$\text{and } \tilde{c}_{2j+1} = \left(\frac{3j\pi}{2}\right)^{\frac{2}{3}} \cdot \left(1 + \frac{13}{18j} + \mathcal{O}\left(\frac{1}{j^2}\right)\right). \quad (56)$$

*Proof:* Let  $j \geq 0$ . Applying (28) with  $x = \tilde{c}_{2j}$ ,

$$2\pi^{\frac{1}{2}}\tilde{c}_{2j}^{-\frac{1}{4}} Ai'(0) \left( \sin(\tilde{\xi}_{2j} - \frac{7\pi}{12})P(\frac{1}{3}, \tilde{\xi}_{2j}) + \cos(\tilde{\xi}_{2j} - \frac{7\pi}{12})Q(\frac{1}{3}, \tilde{\xi}_{2j}) \right) = u(-\tilde{c}_{2j}) = 0.$$

Thus, using Lemma 1 and  $\tilde{\xi}_{2j} > \frac{1}{\sqrt{13}}$  (thanks to  $\tilde{a}_0 > \left(\frac{3}{2\sqrt{13}}\right)^{\frac{2}{3}}$ ), we have

$$P(\frac{1}{3}, \tilde{\xi}_{2j}) > 0 \quad \text{and} \quad \tan\left(\tilde{\xi}_{2j} - \frac{7\pi}{12}\right) = \frac{\sin(\tilde{\xi}_{2j} - \frac{7\pi}{12})}{\cos(\tilde{\xi}_{2j} - \frac{7\pi}{12})} = -\frac{Q(\frac{1}{3}, \tilde{\xi}_{2j})}{P(\frac{1}{3}, \tilde{\xi}_{2j})}. \quad (57)$$

With (32) and (57) we get:

$$\left| \tan\left(\tilde{\xi}_{2j} - \frac{7\pi}{12}\right) \right| < \frac{5}{36 \cdot \tilde{\xi}_{2j}}. \quad (58)$$

From (45) and (58), it leads to

$$\left| \tilde{\xi}_{2j} - \frac{7\pi}{12} - j\pi \right| < \arctan \left( \frac{5}{36 \cdot \tilde{\xi}_{2j}} \right) \leq \frac{5}{36 \cdot \tilde{\xi}_{2j}} \leq \frac{5}{36(j\pi + \frac{\pi}{2})}, \quad (59)$$

which proves the assertion on the interval of localization of  $\tilde{\xi}_{2j}$ .

Since  $\tilde{a}_0 > \left( \frac{3}{2\sqrt{11}} \right)^{\frac{2}{3}}$ ,  $\xi_{2j} > \frac{1}{\sqrt{11}}$  and, using Lemma 1, we have  $P(\frac{2}{3}, \xi_{2j}) > 0$ .

Applying (31) with  $x = c_{2j}$ ,

$$-2\pi^{\frac{1}{2}} c_{2j}^{\frac{1}{2}} Ai(0) \left( -\cos(\xi_{2j} + \frac{\pi}{12}) P(\frac{2}{3}, \xi_{2j}) + \sin(\xi_{2j} + \frac{\pi}{12}) Q(\frac{2}{3}, \xi_{2j}) \right) = v'(-c_{2j}) = 0.$$

Thus,

$$\frac{Q(\frac{2}{3}, \xi_{2j})}{P(\frac{2}{3}, \xi_{2j})} = \cotan \left( \xi_{2j} + \frac{\pi}{12} \right) = -\tan \left( \xi_{2j} + \frac{\pi}{12} - \frac{\pi}{2} \right) = -\tan \left( \xi_{2j} - \frac{5\pi}{12} \right). \quad (60)$$

Using (33) and (60) we get:

$$\left| \tan \left( \xi_{2j} - \frac{5\pi}{12} \right) \right| < \frac{7}{12 \cdot \xi_{2j}}, \quad (61)$$

and the rest of the proof of the interval of localization of  $\xi_{2j}$  is similar to what we have done for  $\tilde{\xi}_{2j}$ , thanks to (44). The intervals of localization of  $\xi_{2j+1}$  and  $\tilde{\xi}_{2j+1}$  are obtained in a similar way.

In order to prove (50), we need a more precise estimate on  $\xi_{2j}$ . Using (60) and [1, 9.2.9 and 9.2.10],

$$\begin{aligned} \tan \left( \xi_{2j} - \frac{5\pi}{12} \right) &= \frac{\frac{7}{72\xi_{2j}} - \frac{7 \times 65 \times 209}{6 \times 8^3 \times 9^3 \xi_{2j}^3} + \mathcal{O} \left( \frac{1}{\xi_{2j}^5} \right)}{1 - \frac{7 \times 65}{2 \times 8^2 \times 9^2 \xi_{2j}^2} + \mathcal{O} \left( \frac{1}{\xi_{2j}^4} \right)} \\ &= \left( \frac{7}{72\xi_{2j}} - \frac{7 \times 65 \times 209}{6 \times 8^3 \times 9^3 \xi_{2j}^3} + \mathcal{O} \left( \frac{1}{\xi_{2j}^5} \right) \right) \left( 1 + \frac{7 \times 65}{2 \times 8^2 \times 9^2 \xi_{2j}^2} + \mathcal{O} \left( \frac{1}{\xi_{2j}^4} \right) \right) \\ &= \frac{7}{72\xi_{2j}} + \mathcal{O} \left( \frac{1}{\xi_{2j}^3} \right). \end{aligned}$$

Thus, thanks to  $\xi_{2j} - \frac{5\pi}{12} - j\pi \in [-\frac{\pi}{12}, \frac{\pi}{12}]$ ,

$$\xi_{2j} - \frac{5\pi}{12} - j\pi = \arctan \left( \frac{7}{72\xi_{2j}} + \mathcal{O} \left( \frac{1}{\xi_{2j}^3} \right) \right) = \frac{7}{72\xi_{2j}} \left( 1 + \mathcal{O} \left( \frac{1}{\xi_{2j}^2} \right) \right).$$

Since  $\xi_{2j} \in [j\pi + \frac{\pi}{3}, j\pi + \frac{\pi}{2}]$ , there exists a constant  $C > 0$  such that:

$$\frac{7}{72(j\pi + \frac{\pi}{2})} \left( 1 - \frac{C}{j^2} \right) \leq \xi_{2j} - \frac{5\pi}{12} - j\pi \leq \frac{7}{72(j\pi + \frac{\pi}{3})} \left( 1 + \frac{C}{j^2} \right)$$

which proves that

$$\xi_{2j} = \frac{5\pi}{12} + j\pi + \frac{7}{72(j\pi + \frac{\pi}{2})} + \mathcal{O} \left( \frac{1}{j^3} \right).$$

Since  $c_{2j} = \left(\frac{3}{2}\xi_{2j}\right)^{\frac{2}{3}}$ ,

$$\begin{aligned} c_{2j} &= \left(\frac{3j\pi}{2} + \frac{5\pi}{8} + \frac{7}{48(j\pi + \frac{\pi}{2})} + \mathcal{O}\left(\frac{1}{j^3}\right)\right)^{\frac{2}{3}} \\ &= \left(\frac{3j\pi}{2}\right)^{\frac{2}{3}} \cdot \left(1 + \frac{5}{12j} + \frac{7}{72j\pi(j\pi + \frac{\pi}{2})} + \mathcal{O}\left(\frac{1}{j^4}\right)\right)^{\frac{2}{3}} \\ &= \left(\frac{3j\pi}{2}\right)^{\frac{2}{3}} \cdot \left(1 + \frac{5}{18j} + \frac{7}{48j\pi(j\pi + \frac{\pi}{2})} - \frac{1}{9}\left(\frac{5}{12j}\right)^2 + \mathcal{O}\left(\frac{1}{j^4}\right)\right) \\ &= \left(\frac{3j\pi}{2}\right)^{\frac{2}{3}} \cdot \left(1 + \frac{5}{18j} + \mathcal{O}\left(\frac{1}{j^2}\right)\right), \end{aligned}$$

which proves (50). Similarly, using  $\tilde{\xi}_{2j} \in (j\pi + \frac{\pi}{2}, j\pi + \frac{2\pi}{3})$ ,  $\xi_{2j+1} \in (j\pi + \frac{5\pi}{6}, j\pi + \pi)$  and  $\tilde{\xi}_{2j+1} \in (j\pi + \pi, j\pi + \frac{7\pi}{6})$ , one proves (54), (52) and (56).  $\square$

**Remark.** From the proof of the asymptotic expansions of  $c_k$  and  $\tilde{c}_k$ , one could obtain asymptotic expansion of these sequences at any order, using the developments of the functions  $P$  and  $Q$  ([1, 9.2.9 and 9.2.10]). One would then get similar formula as those for the zeroes of the functions  $Ai$ ,  $Ai'$ ,  $Bi$  and  $Bi'$  ([1, 10.4.94 and below]).

## 5. PRELIMINARIES TO THE COMPUTATION OF THE BAND EDGES

**5.1. Characterization of the spectral band edges.** The band edges are characterized by the functions  $U_\theta$ ,  $V_\theta$  and their derivatives, through the equations (26) and (27).

To find the band edges  $E_{\min}^k$  and  $E_{\max}^k$  for any  $k \geq 0$ , we have to solve the four equations:

$$U'_\theta(L_0) = u'(-\theta V_0 - \theta E)v'(-\theta E) - v'(-\theta V_0 - \theta E)u'(-\theta E) = 0, \quad (62)$$

$$V_\theta(L_0) = u(-\theta E)v(-\theta V_0 - \theta E) - v(-\theta E)u(-\theta V_0 - \theta E) = 0, \quad (63)$$

$$U_\theta(L_0) = v(-\theta E)u'(-\theta V_0 - \theta E) - u(-\theta E)v'(-\theta V_0 - \theta E) = 0, \quad (64)$$

$$V'_\theta(L_0) = v'(-\theta E)u(-\theta V_0 - \theta E) - u'(-\theta E)v(-\theta V_0 - \theta E) = 0. \quad (65)$$

We have the four equivalences:

$$(1) \text{ for } \theta E \notin \{\tilde{c}_{2j+1} - \theta V_0\}_{j \geq 0} \cup \{\tilde{c}_{2j+1}\}_{j \geq 0},$$

$$u'(-\theta V_0 - \theta E)v'(-\theta E) - v'(-\theta V_0 - \theta E)u'(-\theta E) = 0 \Leftrightarrow \frac{v'(-\theta V_0 - \theta E)}{u'(-\theta V_0 - \theta E)} = \frac{v'(-\theta E)}{u'(-\theta E)},$$

$$(2) \text{ for } \theta E \notin \{\tilde{c}_{2j} - \theta V_0\}_{j \geq 0} \cup \{\tilde{c}_{2j}\}_{j \geq 0},$$

$$u(-\theta E)v(-\theta V_0 - \theta E) - v(-\theta E)u(-\theta V_0 - \theta E) = 0 \Leftrightarrow \frac{v(-\theta V_0 - \theta E)}{u(-\theta V_0 - \theta E)} = \frac{v(-\theta E)}{u(-\theta E)},$$

$$(3) \text{ for } \theta E \notin \{\tilde{c}_{2j+1} - \theta V_0\}_{j \geq 0} \cup \{\tilde{c}_{2j}\}_{j \geq 0},$$

$$u(-\theta E)v'(-\theta V_0 - \theta E) - v(-\theta E)u'(-\theta V_0 - \theta E) = 0 \Leftrightarrow \frac{v'(-\theta V_0 - \theta E)}{u'(-\theta V_0 - \theta E)} = \frac{v'(-\theta E)}{u'(-\theta E)},$$



$$(4) \text{ for } \theta E \notin \{\tilde{c}_{2j} - \theta V_0\}_{j \geq 0} \cup \{\tilde{c}_{2j+1}\}_{j \geq 0},$$

$$u'(-\theta E)v(-\theta V_0 - \theta E) - v'(-\theta E)u(-\theta V_0 - \theta E) = 0 \Leftrightarrow \frac{v(-\theta V_0 - \theta E)}{u(-\theta V_0 - \theta E)} = \frac{v'(-\theta E)}{u'(-\theta E)}.$$

We look at the cases where the conditions on  $-\theta V_0 - \theta E$  and  $-\theta E$  are not satisfied. The semiclassical parameter  $\theta V_0$  is the parameter for the problem studied. Under this observation, assume that:

$$\theta V_0 \in \{\tilde{c}_p - \tilde{c}_q, \mid p > q \geq 0\} := \mathbf{Z}.$$

Then, for  $\theta V_0 = \tilde{c}_p - \tilde{c}_q \in \mathbf{Z}$ , in the set of values of  $c_k$  and  $\tilde{c}_k$ ,  $\theta E = \tilde{c}_q$  is the unique solution of the equation (62) if  $p$  and  $q$  are odd, (63) if  $p$  and  $q$  are even, (64) if  $p$  is odd and  $q$  is even and (65) if  $p$  is even and  $q$  is odd.

Conversely, if  $\theta V_0 \notin \mathbf{Z}$ , then none of the  $\tilde{c}_k$  is a solution in  $-\theta E$  of any of the equations (62), (63), (64) and (65).

**Assumption.** From now on, we assume that  $\theta V_0 \notin \mathbf{Z}$ .

Note that, however, all our results hold true when  $\theta V_0 \in \mathbf{Z}$ , this assumption is only made for convenience's sake.

Since we have the four equivalences above, the band edges of the spectral bands of  $H$  are solutions of the four following equations:

$$\frac{v'}{u'}(-\theta V_0 - \theta E) = \frac{v'}{u'}(-\theta E), \text{ for } \theta E \notin \{\tilde{c}_{2j+1} - \theta V_0\}_{j \geq 0} \cup \{\tilde{c}_{2j+1}\}_{j \geq 0}, \quad (66)$$

$$\frac{v}{u}(-\theta V_0 - \theta E) = \frac{v}{u}(-\theta E), \text{ for } \theta E \notin \{\tilde{c}_{2j} - \theta V_0\}_{j \geq 0} \cup \{\tilde{c}_{2j}\}_{j \geq 0}, \quad (67)$$

$$\frac{v'}{u'}(-\theta V_0 - \theta E) = \frac{v}{u}(-\theta E), \text{ for } \theta E \notin \{\tilde{c}_{2j+1} - \theta V_0\}_{j \geq 0} \cup \{\tilde{c}_{2j}\}_{j \geq 0}, \quad (68)$$

$$\frac{v}{u}(-\theta V_0 - \theta E) = \frac{v'}{u'}(-\theta E), \text{ for } \theta E \notin \{\tilde{c}_{2j} - \theta V_0\}_{j \geq 0} \cup \{\tilde{c}_{2j+1}\}_{j \geq 0}. \quad (69)$$

**5.2. Variations of  $\frac{v}{u}$  and  $\frac{v'}{u'}$ .** Using the value of the Wronskian of  $u$  and  $v$  one has:

$$\forall x \in [0, +\infty), \left(\frac{v}{u}\right)'(x) = \frac{v'(x)u(x) - v(x)u'(x)}{u^2(x)} = \frac{1}{u^2(x)} > 0$$

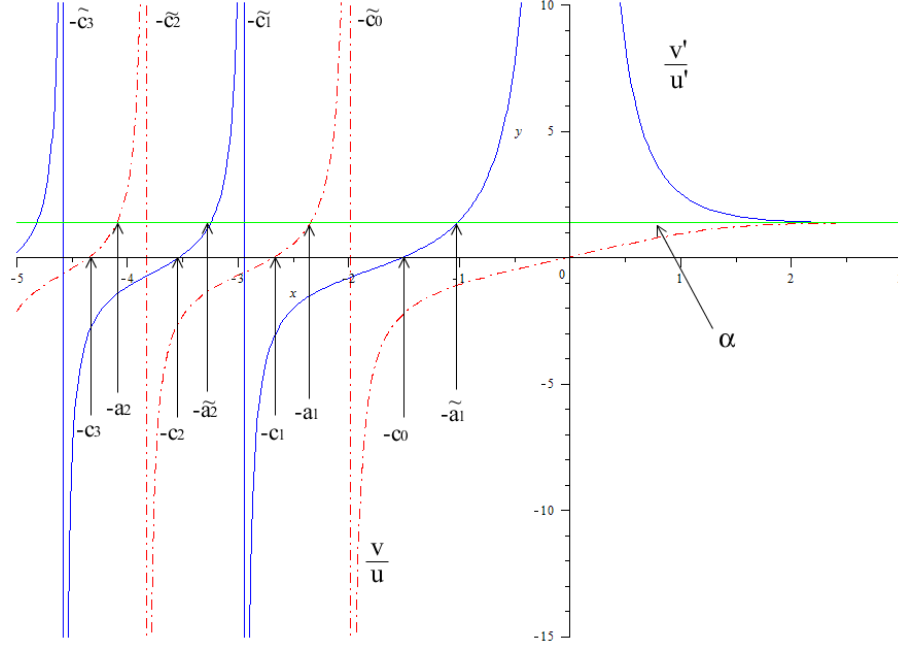
and

$$\forall x \in (0, +\infty), \left(\frac{v'}{u'}\right)'(x) = \frac{xv(x)u'(x) - xv'(x)u(x)}{(u'(x))^2} = -\frac{x}{(u'(x))^2} < 0.$$

Thus, the functions  $\frac{v}{u}$  and  $\frac{v'}{u'}$  have the following behaviour. Let  $j \geq 0$ .

- On every interval  $(-\tilde{c}_{2j+2}, -\tilde{c}_{2j})$ , the function  $\frac{v}{u}$  is continuous, strictly increasing and is a bijection from  $(-\tilde{c}_{2j+2}, -\tilde{c}_{2j})$  to  $\mathbb{R}$ . We also have that  $\frac{v}{u}$  is continuous, strictly increasing and is a bijection from  $(-\tilde{c}_0, +\infty)$  to  $(-\infty, \alpha)$ .
- On every interval  $(-\tilde{c}_{2j+3}, -\tilde{c}_{2j+1})$ , the function  $\frac{v'}{u'}$  is continuous, strictly increasing and is a bijection from  $(-\tilde{c}_{2j+3}, -\tilde{c}_{2j+1})$  to  $\mathbb{R}$ . We also have that  $\frac{v'}{u'}$  is continuous and strictly increasing on  $(-\tilde{c}_1, 0)$  from  $-\infty$  to  $+\infty$ . It is also continuous, strictly decreasing and a bijection from  $(0, +\infty)$  to  $(\alpha, +\infty)$ .

We remark that  $\alpha$  is the common limit at infinity of the two functions  $\frac{v}{u}$  and  $\frac{v'}{u'}$ , thanks to the limits  $\frac{Bi(x)}{Ai(x)} \xrightarrow{x \rightarrow +\infty} +\infty$  and  $\frac{Bi'(x)}{Ai'(x)} \xrightarrow{x \rightarrow +\infty} -\infty$ .



**5.3. Some auxiliary functions.** One sets, for  $x \geq 0$  and  $z \in \mathbb{R}$ ,

$$f_x(z) = v'(x-z)u(x) - u'(x-z)v(x) = \pi (Bi'(x-z)Ai(x) - Ai'(x-z)Bi(x)) \quad (70)$$

and

$$g_x(z) = v(x-z)u(x) - u(x-z)v(x) = \pi (Bi(x-z)Ai(x) - Ai(x-z)Bi(x)). \quad (71)$$

The expressions in terms of the classical Airy functions allow us to use classical properties of the  $Ai$  and  $Bi$  functions instead of the properties of  $u$  and  $v$  when it makes proofs easier.

The functions  $f_x$  and  $g_x$  are non-zero solutions of differential equations which satisfy the assumptions of Sturm's theorem, thus their zeroes are isolated on the real line. We denote by

$$z_0(x) < z_2(x) < \dots < z_{2j}(x) < \dots$$

the zeroes of  $f_x$  arranged in increasing order. Then, since 0 is the first zero of  $g_x$  for every  $x$ , we denote by

$$0 < z_1(x) < z_3(x) < \dots < z_{2j+1}(x) < \dots$$

the zeroes of  $g_x$  arranged in increasing order.

We can characterize these zeroes and prove that none of them is negative.

Let  $j \geq 0$  an integer. Let  $x \geq 0$  and denote by  $\psi_{2j}(x)$  the unique solution of the equation

$$\frac{v'}{u'}(z) = \frac{v}{u}(x), \quad z \in [-c_{2j}, -\tilde{a}_{j+1}]. \quad (72)$$

We also denote by  $\psi_{2j+1}(x)$  the unique solution of the equation

$$\frac{v}{u}(z) = \frac{v}{u}(x), \quad z \in [-c_{2j+1}, -a_{j+1}]. \quad (73)$$

**Lemma 3.** *For every  $k \geq 0$ , the function  $\psi_k$  is well defined, continuous and strictly increasing.*

*Proof:* Let  $j \geq 0$ . The function  $\frac{v'}{u'}$  is a bijection from  $[-c_{2j}, -\tilde{a}_{j+1})$  to  $[0, \alpha)$  and we denote by

$$\left(\frac{v'}{u'}\right)_{2j}^{-1} : [0, \alpha) \rightarrow [-c_{2j}, -\tilde{a}_{j+1})$$

its reciprocal function. Since for every  $x \geq 0$ ,  $\frac{v}{u}(x) \in [0, \alpha)$ , we have:

$$\forall x \geq 0, \quad \psi_{2j}(x) = \left(\frac{v'}{u'}\right)_{2j}^{-1} \left(\frac{v}{u}(x)\right).$$

Thus, the function  $\psi_{2j}$  is well defined and it is continuous by continuity of  $\frac{v}{u}$  on  $[0, +\infty)$  and of the inverse of  $\frac{v'}{u'}$  on  $[0, \alpha)$ . Since  $\frac{v'}{u'}$  is strictly increasing on  $[-c_{2j}, -\tilde{a}_{j+1})$ , its reciprocal function is strictly increasing on  $[0, \alpha)$  and since  $\frac{v}{u}$  is strictly increasing on  $[0, +\infty)$ , we deduce that  $\psi_{2j}$  is strictly increasing on  $[0, +\infty)$ . The function  $\frac{v}{u}$  is a bijection from  $(-c_{2j+1}, -a_{j+1}]$  to  $[0, \alpha)$  and we denote by

$$\left(\frac{v}{u}\right)_{2j+1}^{-1} : [0, \alpha) \rightarrow [-c_{2j+1}, -a_{j+1}]$$

its reciprocal function. With the same arguments as before, we have that

$$\forall x \geq 0, \quad \psi_{2j+1}(x) = \left(\frac{v}{u}\right)_{2j+1}^{-1} \left(\frac{v}{u}(x)\right)$$

and thus  $\psi_{2j+1}$  is well defined, continuous and strictly increasing.  $\square$

**Lemma 4.** *Let  $k \geq 0$ . Then, for every  $x \geq 0$ ,*

$$z_k(x) \geq 0 \quad \text{and} \quad z_k(x) = x - \psi_k(x).$$

*Therefore,  $z_k$  is continuous on  $[0, +\infty)$ . Moreover, for every  $k \geq 0$ , the function  $z_k$  is strictly increasing from  $[0, +\infty)$  to  $[c_k, +\infty)$ .*

This result is proven in Appendix B.

Let  $j \geq 0$ . For  $x \geq 0$ , denote by  $\psi^{2j}(x) \in (-a_{j+1}, -\tilde{c}_{2j}]$  the unique solution of the equation

$$\frac{v}{u}(z) = \frac{v'}{u'}(x), \quad z \in (-a_{j+1}, -\tilde{c}_{2j}]. \quad (74)$$

We also denote by  $\psi^{2j+1}(x) \in (-\tilde{a}_{j+2}, -\tilde{c}_{2j+1})$  the unique solution of the equation

$$\frac{v'}{u'}(z) = \frac{v'}{u'}(x), \quad z \in (-\tilde{a}_{j+2}, -\tilde{c}_{2j+1}). \quad (75)$$

**Lemma 5.** *For every  $k \geq 0$ , the function  $\psi^k$  is well defined, continuous and strictly decreasing on  $[0, +\infty)$ .*

*Proof:* We assume that  $k$  is even,  $k = 2j$  for one  $j \geq 0$ . The function  $\frac{v}{u}$  is a continuous bijection from  $(-a_{j+1}, -\tilde{c}_{2j})$  to  $[\alpha, +\infty)$  and we denote its reciprocal function by

$$\left(\frac{v}{u}\right)_{2j}^{-1} : [\alpha, +\infty) \rightarrow (-a_{j+1}, -\tilde{c}_{2j}).$$

Since for every  $x \geq 0$ ,  $\frac{v'}{u'}(x) \in [\alpha, +\infty)$ , we have:

$$\forall x \geq 0, \psi^{2j}(x) = \left(\frac{v}{u}\right)_{2j}^{-1} \left(\frac{v'}{u'}(x)\right).$$

Then  $\psi^{2j}$  is well defined, continuous and it is the unique solution of (74). Moreover,  $\left(\frac{v}{u}\right)_{2j}^{-1}$  is a strictly increasing function from  $[\alpha, +\infty)$  to  $(-a_{j+1}, -\tilde{c}_{2j})$  and  $\frac{v'}{u'}$  is strictly decreasing on  $[0, +\infty)$ . Thus,  $\psi^{2j}$  is strictly decreasing on  $[0, +\infty)$ .

We assume that  $k$  is odd,  $k = 2j + 1$  for one  $j \geq 0$ . The function  $\frac{v'}{u'}$  is a continuous bijection from  $(-\tilde{a}_{j+2}, -\tilde{c}_{2j+1})$  to  $[\alpha, +\infty)$  and we denote its reciprocal function by

$$\left(\frac{v'}{u'}\right)_{2j+1}^{-1} : [\alpha, +\infty) \rightarrow (-\tilde{a}_{j+2}, -\tilde{c}_{2j+1}).$$

Since for every  $x \geq 0$ ,  $\frac{v'}{u'}(x) \in [\alpha, +\infty)$ , we can write:

$$\forall x \geq 0, \psi^{2j+1}(x) = \left(\frac{v'}{u'}\right)_{2j+1}^{-1} \left(\frac{v'}{u'}(x)\right).$$

Then  $\psi^{2j+1}$  is well defined, continuous and it is the unique solution of (75). Moreover,  $\left(\frac{v'}{u'}\right)_{2j+1}^{-1}$  is a strictly increasing function from  $[\alpha, +\infty)$  to  $(-\tilde{a}_{j+2}, -\tilde{c}_{2j+1})$  and  $\frac{v'}{u'}$  is strictly decreasing on  $[0, +\infty)$ . Thus,  $\psi^{2j+1}$  is strictly decreasing on  $[0, +\infty)$ .  $\square$

## 6. THE FIRST SPECTRAL BAND

**6.1. Lower bound of the continuous spectrum.** For values of  $E$  such that  $\theta E < -\theta V_0$ , we show that there is no solutions to equations (66), (67), (69) and (68) which is natural, from a physical point of view, since in this case, the energy is smaller than the minimum of the potential and it is as if the potential was not “seen” at this energy.

**Proposition 5.** *For every  $\theta V_0 \geq 0$ ,  $\sigma(H) \subset [-V_0, +\infty)$ .*

*Proof:* We remark that on the interval  $[0, +\infty)$ ,  $\frac{v}{u} < \alpha$  and  $\frac{v'}{u'} > \alpha$ . Thus, these two functions cannot have a common value on this interval and equations (69) and (68) do not have any solution with  $0 < -\theta V_0 - \theta E < -\theta E$ .

Moreover, we already know that  $\frac{v}{u}$  is strictly increasing on  $[0, +\infty)$  and  $\frac{v'}{u'}$  is strictly decreasing on  $(0, +\infty)$ . Since  $-\theta V_0 - \theta E \neq -\theta E$  the equations (66), (67) do not have any solution when  $0 < -\theta V_0 - \theta E < -\theta E$ .  $\square$

**Remark.** This result holds for every  $\theta V_0$  strictly positive. In particular we do not need to assume this semiclassical parameter to be large.

**6.2. The bottom of the spectrum.** At first, we determine the bottom of the spectrum. It has to be a solution of either the equation (66) or the equation (67) with  $-\theta E \geq 0$  and thus  $-\theta V_0 - \theta E < 0$ .

We start by proving that for every  $\theta V_0 > 0$ , the equation (66) has a unique solution with  $-\theta E > 0$  and  $-\theta V_0 - \theta E \in [-\tilde{a}_1, 0)$ . The function  $\frac{v'}{u'}$  is an increasing continuous bijection from  $(-\tilde{a}_1, 0)$  to  $[\alpha, +\infty)$  and thus, since for every  $x > 0$ ,  $\frac{v'}{u'}(x) \in [\alpha, +\infty)$ , one can define:

$$\forall x > 0, \psi(x) = \left( \frac{v'}{u'} \Big|_{(-\tilde{a}_1, 0)} \right)^{-1} \left( \frac{v'}{u'}(x) \right). \quad (76)$$

The function  $\psi$  does not belong to the family of the functions  $\psi_{2k+1}$ , due to the difference of behaviour of  $\frac{v'}{u'}$  on  $(-\tilde{a}_1, +\infty)$  compared to  $(-\infty, -\tilde{a}_1)$ .

The function  $\psi$  is a continuous decreasing bijection from  $(0, +\infty)$  to  $(-\tilde{a}_1, 0)$  and  $x \mapsto x - \psi(x)$  is a continuous increasing bijection from  $(0, +\infty)$  to  $(0, +\infty)$ . Thus,

$$\forall \theta V_0 > 0, \exists! \tilde{x} > 0, \tilde{x} - \psi(\tilde{x}) = \theta V_0.$$

One sets  $\tilde{E} = -\frac{\tilde{x}}{\theta}$  and since  $\tilde{x} = \theta V_0 + \psi(\tilde{x}) \in (-\tilde{a}_1 + \theta V_0, \theta V_0)$  one has

$$-V_0 < \tilde{E} < -V_0 + \frac{\tilde{a}_1}{\theta}. \quad (77)$$

We remark that  $\tilde{E}$  is the smallest solution of (66).

Now we turn to the smallest solution of (67). Since the function  $z_1$  is an increasing continuous bijection from  $[0, +\infty)$  to  $[c_1, +\infty)$ ,

$$\forall \theta V_0 \geq c_1, \exists! x_1 \geq 0, z_1(x_1) = x_1 - \psi_1(x_1) = \theta V_0.$$

One sets  $\check{E}_1 = -\frac{x_1}{\theta}$  and since  $x_1 = \theta V_0 + \psi_1(x_1) \in (-c_1 + \theta V_0, -a_1 + \theta V_0)$  one has

$$-V_0 + \frac{a_1}{\theta} < \check{E}_1 < -V_0 + \frac{c_1}{\theta}.$$

Since  $\tilde{a}_1 < a_1$  we have  $\tilde{E} < \check{E}_1$  and thus  $E_{\min}^0 = \tilde{E}$ . In particular,  $E_{\min}^0$  is the smallest solution of (66). Moreover, it is the smallest solution among those of (66) and (67).

Now that we have identified the bottom of the spectrum of  $H$  as the smallest solution among the possible solutions of (66) and (67), we can prove the estimates stated in Theorem 3.

*Proof:* (of Theorem 3).

(1) Since  $E_{\min}^0 = \tilde{E}$ , by (77) we have, for every  $\theta V_0 > 0$ ,  $-\theta V_0 < \theta E_{\min}^0 < -\theta V_0 + \tilde{a}_1$ .

Let  $\theta V_0 > 0$ . By the previous inequality,  $-\theta E_{\min}^0 \in (-\tilde{a}_1 + \theta V_0, \theta V_0)$ . We recall that, since  $u$  and  $v$  are linear combinations of  $Ai$  and  $Bi$  and since  $E_{\min}^0$  is a solution of (66), it also satisfies:

$$\frac{Bi'}{Ai'}(-\theta E_{\min}^0 - \theta V_0) = \frac{Bi'}{Ai'}(-\theta E_{\min}^0), \quad -\theta E_{\min}^0 - \theta V_0 \in (-\tilde{a}_1, 0).$$

We introduce the functions

$$F_{\pm}(\cdot, \theta V_0) : \begin{array}{l} I_{\pm} \rightarrow \mathbb{R} \\ x \mapsto \frac{Bi'}{Ai'}\left(x - \frac{\theta V_0}{2}\right) - \frac{Bi'}{Ai'}\left(x + \frac{\theta V_0}{2}\right) \end{array}$$

with  $I_- = (-\frac{\theta V_0}{2}, \frac{\theta V_0}{2})$  and  $I_+ = (-\tilde{a}_1 + \frac{\theta V_0}{2}, \frac{\theta V_0}{2})$ . We remark that, for every  $\theta V_0 > 0$ , the unique zero of  $F_{\pm}(\cdot, \theta V_0)$  on  $I_{\pm}$  is  $-\theta E_{\min}^0 - \frac{\theta V_0}{2}$ .

Thanks to the fact that 0 is the point of maximum of  $\frac{Bi'}{Ai'}$  on  $(-\tilde{a}_1, +\infty)$ , one has:

$$F_{\pm}\left(\frac{\theta V_0}{2}, \theta V_0\right) = \frac{Bi'}{Ai'}(0) - \frac{Bi'}{Ai'}(\theta V_0) > 0.$$

*First case:*  $\theta V_0 \geq 2\tilde{a}_1$ . In this case,  $-\tilde{a}_1 + \frac{\theta V_0}{2} > 0$  hence the unique zero of  $F_+(\cdot, \theta V_0)$  on  $I_+$  is strictly positive, hence  $-\theta E_{\min}^0 - \frac{\theta V_0}{2} > 0$  which implies that  $E_{\min}^0 < -\frac{V_0}{2}$ . Thus, point (1) is proved for every  $\theta V_0 \geq 2\tilde{a}_1$ .

*Second case:*  $0 < \theta V_0 < 2\tilde{a}_1$ . We want to prove that the unique zero of  $F_{\pm}(\cdot, \theta V_0)$  on  $I_{\pm}$  is strictly positive. Since  $F_{\pm}(\frac{\theta V_0}{2}, \theta V_0) > 0$ , it is sufficient to prove that  $F_{\pm}(0, \theta V_0) < 0$ . Indeed, if  $0 < \theta V_0 < \tilde{a}_1$ , then  $0 \in I_-$  and we study the unique zero of  $F_-$  in  $I_-$ . If  $\tilde{a}_1 \leq \theta V_0 < 2\tilde{a}_1$ , then  $-\tilde{a}_1 + \frac{\theta V_0}{2} < 0$  and  $0 \in I_+$ . In this case, we study the unique zero of  $F_+$  in  $I_+$ .

We have:

$$F_{\pm}(0, \theta V_0) = \frac{Bi'}{Ai'}\left(-\frac{\theta V_0}{2}\right) - \frac{Bi'}{Ai'}\left(\frac{\theta V_0}{2}\right).$$

Let  $y = \frac{\theta V_0}{2}$  so that  $y \in (0, \tilde{a}_1)$  and set:

$$\forall y \in (0, \tilde{a}_1), G(y) = \frac{Bi'}{Ai'}(-y) - \frac{Bi'}{Ai'}(y).$$

One has, for every  $y \in (0, \tilde{a}_1)$ ,

$$G'(y) = \frac{y}{\pi(Ai'(-y))^2(Ai'(y))^2} ((Ai'(-y) - Ai'(y))(Ai'(-y) + Ai'(y))).$$

On  $(0, \tilde{a}_1)$ ,  $\frac{y}{\pi(Ai'(-y))^2(Ai'(y))^2} > 0$  and as  $Ai'$  is negative on  $(-\tilde{a}_1, +\infty)$ ,  $Ai'(-y) + Ai'(y) < 0$  for every  $y \in (0, \tilde{a}_1)$ .

Let

$$K : \begin{array}{ll} (0, \tilde{a}_1) & \rightarrow \mathbb{R} \\ y & \mapsto Ai'(-y) - Ai'(y) \end{array}.$$

Then  $K(0) = 0$  and

$$\forall y \in (0, \tilde{a}_1), K'(y) = -Ai''(-y) - Ai''(y) = y(Ai(-y) - Ai(y)).$$

But, the Airy function  $Ai$  is decreasing on  $(-\tilde{a}_1, +\infty)$  hence, for  $y \in (0, \tilde{a}_1)$ ,  $Ai(-y) - Ai(y) > 0$  and  $K'(y) > 0$ . Thus,  $K$  is strictly increasing on  $(0, \tilde{a}_1)$  and

$$\forall y \in (0, \tilde{a}_1), K(y) > K(0) = 0.$$

Thus, for every  $y \in (0, \tilde{a}_1)$ ,  $G'(y) < 0$ . Since  $G(0) = 0$ , for every  $y \in (0, \tilde{a}_1)$ ,  $G(y) < 0$ , which rewrites

$$\forall \theta V_0 \in (0, 2\tilde{a}_1), F_{\pm}(0, \theta V_0) < 0.$$

Thus, the unique zero of  $F_{\pm}(\cdot, \theta V_0)$  in  $I_{\pm}$  is strictly positive. Thus,  $-\theta E_{\min}^0 - \frac{\theta V_0}{2} \in (0, \frac{\theta V_0}{2})$  and  $\theta E_{\min}^0 < -\frac{\theta V_0}{2}$ .

Taking in account the result in both cases, point (1) is proved.

(2) Since  $E_{\min}^0$  is the smallest solution of (66), if one sets  $X = -\theta E_{\min}^0 - \theta V_0 + \tilde{a}_1$ , then  $X$  satisfies

$$\frac{v'}{u'}(X - \tilde{a}_1) = \frac{v'}{u'}(X + \theta V_0 - \tilde{a}_1), \quad X \in [0, \tilde{a}_1]. \quad (78)$$

Since  $x \mapsto x - \psi(x)$  is increasing on  $(0, +\infty)$ , when  $\theta V_0$  tends to infinity,  $X - \tilde{a}_1$  tends to  $-\tilde{a}_1$  and  $X + \theta V_0 - \tilde{a}_1$  tends to  $+\infty$ . Therefore, both members of (78) tends to  $\alpha$  when  $\theta V_0$  tends to  $+\infty$ . We assume that  $\theta V_0 > \tilde{a}_1$ .

Using [1, 10.4.61, 10.4.66] in the equality (78), one gets

$$\frac{v'}{u'}(X - \tilde{a}_1) = \alpha + \alpha\sqrt{3}e^{-\frac{4}{3}(X+\theta V_0-\tilde{a}_1)^{\frac{3}{2}}} \left(1 + \mathcal{O}\left((X + \theta V_0 - \tilde{a}_1)^{-\frac{3}{2}}\right)\right). \quad (79)$$

Let  $\epsilon = e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_1)^{\frac{3}{2}}}$ , which amounts to  $\theta V_0 - \tilde{a}_1 = \left(-\frac{3}{4}\ln(\epsilon)\right)^{\frac{2}{3}}$ . In particular,  $\theta V_0$  tends to  $+\infty$  if and only if  $\epsilon$  tends to  $0^+$ .

We use the following identity valid for strictly positive real numbers  $a$  and  $b$ :

$$a^{\frac{3}{2}} - b^{\frac{3}{2}} - \frac{3}{2}b^{\frac{1}{2}}(a - b) = (a - b)^2 \frac{2\sqrt{\frac{a}{b}} + 1}{2\left(\sqrt{\frac{a}{b}} + 1\right)^2} b^{-\frac{1}{2}} \quad (80)$$

with  $a = X + \theta V_0 - \tilde{a}_1 = \epsilon Y + \theta V_0 - \tilde{a}_1$  and  $b = \theta V_0 - \tilde{a}_1 = \left(-\frac{3}{4}\ln(\epsilon)\right)^{\frac{2}{3}}$ . Then,

$$-\frac{4}{3}(X + \theta V_0 - \tilde{a}_1)^{\frac{3}{2}} + \frac{4}{3}\left(\left(-\frac{3}{4}\ln(\epsilon)\right)^{\frac{2}{3}}\right)^{\frac{3}{2}} + 2\left(-\frac{3}{4}\ln(\epsilon)\right)^{\frac{1}{3}}\epsilon Y = \left(-\frac{3}{4}\ln(\epsilon)\right)^{-\frac{1}{3}}(\epsilon Y)^2 Q(\epsilon, Y)$$

where

$$Q(\epsilon, Y) = \frac{4}{3} \frac{2\left(\frac{\epsilon Y + \theta V_0 - \tilde{a}_1}{\left(-\frac{3}{4}\ln(\epsilon)\right)^{\frac{1}{3}}}\right)^{\frac{1}{2}} + 1}{2\left(\left(\frac{\epsilon Y + \theta V_0 - \tilde{a}_1}{\left(-\frac{3}{4}\ln(\epsilon)\right)^{\frac{1}{3}}}\right)^{\frac{1}{2}} + 1\right)^2}.$$

The condition  $\theta V_0 > \tilde{a}_1$  implies  $0 < \epsilon \leq 1$  and since  $\epsilon Y + \theta V_0 - \tilde{a}_1 = -\theta E_{\min}^0 > 0$ ,

$$\frac{(\epsilon Y + \theta V_0 - \tilde{a}_1)^{\frac{1}{2}}}{\left(-\frac{3}{4}\ln(\epsilon)\right)^{\frac{1}{3}}} \geq 0.$$

If  $\varphi : \mathbb{R}_+ \rightarrow \mathbb{R}$  is defined by  $\varphi(x) = \frac{2x+1}{2(x+1)^2}$  for every  $x \in \mathbb{R}_+$ , then  $\varphi$  is decreasing on  $\mathbb{R}_+$ ,  $\varphi(0) = \frac{1}{2}$  and  $\varphi$  tends to 0 when  $x$  tends to  $+\infty$ . Thus, for every  $\epsilon$  and  $Y$ ,

$$0 < Q(\epsilon, Y) \leq \frac{2}{3}.$$

We have,

$$e^{-\frac{4}{3}(X+\theta V_0-\tilde{a}_1)^{\frac{3}{2}}} = \epsilon \cdot e^{-2\left(-\frac{3}{4}\ln(\epsilon)\right)^{\frac{1}{3}}\epsilon Y + \left(-\frac{3}{4}\ln(\epsilon)\right)^{-\frac{1}{3}}(\epsilon Y)^2 Q(\epsilon, Y)}. \quad (81)$$

The condition  $X \in [0, \tilde{a}_1]$  implies that

$$\left(-\frac{3}{4}\ln(\epsilon)\right)^{\frac{2}{3}} = -\tilde{a}_1 + \theta V_0 \leq X + \theta V_0 - \tilde{a}_1 \leq \tilde{a}_1 + \left(-\frac{3}{4}\ln(\epsilon)\right)^{\frac{2}{3}}$$

and in particular,  $X + \theta V_0 - \tilde{a}_1$  tends to  $+\infty$  when  $\theta V_0$  tends to  $+\infty$ . Moreover,

$$\left(\left(\frac{3}{4}\right)^{\frac{2}{3}} + \frac{\tilde{a}_1}{|\ln(\epsilon)|^{\frac{2}{3}}}\right)^{-\frac{3}{2}} \frac{1}{|\ln(\epsilon)|} \leq (X + \theta V_0 - \tilde{a}_1)^{-\frac{3}{2}} \leq \frac{4}{3} \frac{1}{|\ln(\epsilon)|}.$$

Using (79) and the identity  $\alpha = \frac{v'}{u'}(-\tilde{a}_1)$ , which comes directly from the expressions of  $u$  and  $v$  in terms of  $Ai$  and  $Bi$ , one gets:

$$\begin{aligned} & \frac{1}{\epsilon} \left( \frac{v'}{u'}(\epsilon Y - \tilde{a}_1) - \frac{v'}{u'}(-\tilde{a}_1) \right) = \\ & \alpha \sqrt{3} e^{-2(-\frac{3}{4} \ln(\epsilon))^{\frac{1}{3}} \epsilon Y} e^{(-\frac{3}{4} \ln(\epsilon))^{-\frac{1}{3}} (\epsilon Y)^2 Q(\epsilon, Y)} \left( 1 + \mathcal{O} \left( \frac{1}{|\ln(\epsilon)|} \right) \right). \end{aligned} \quad (82)$$

To estimate the left member of (82) one uses:

$$\frac{v'}{u'}(\epsilon Y - \tilde{a}_1) - \frac{v'}{u'}(-\tilde{a}_1) = \int_0^1 \left( \frac{v'}{u'} \right)' (-\tilde{a}_1 + t\epsilon Y) \epsilon Y dt = \int_0^1 \frac{\tilde{a}_1 - t\epsilon Y}{(u'(-\tilde{a}_1 + t\epsilon Y))^2} \epsilon Y dt.$$

Recall that the strictly decreasing and continuous function  $\psi$  has been introduced in (76) and that, if we denote by  $z$  the function defined on  $(0, +\infty)$  by  $z(x) = x - \psi(x)$ , then  $z$  is a strictly increasing and continuous function. Since for every  $\theta V_0 > 0$ ,  $-\theta E_{\min}^0 = z^{-1}(\theta V_0)$ ,  $\theta V_0 \mapsto -\theta E_{\min}^0(\theta V_0)$  is strictly increasing on  $(0, +\infty)$  and  $\varphi : \theta V_0 \mapsto \psi(-\theta E_{\min}^0(\theta V_0))$  is strictly decreasing and continuous on  $(0, +\infty)$ . Since for every  $\theta V_0 > 0$ ,  $X = \varphi(\theta V_0) + \tilde{a}_1$ , if one assume that  $\theta V_0 \geq \varphi^{-1}(\frac{\tilde{a}_1}{2})$ , then  $X \in [0, \frac{1}{2}\tilde{a}_1]$ .

Thus, for every  $t \in [0, 1]$ ,  $-\tilde{a}_1 + t\epsilon Y \in [-\tilde{a}_1, -\frac{1}{2}\tilde{a}_1]$ . Since  $x \mapsto -\frac{x}{(u'(x))^2}$  is strictly positive and continuous on the interval  $[-\tilde{a}_1, -\frac{1}{2}\tilde{a}_1]$  it is bounded from below by a constant  $C_1 > 0$  and

$$\left| \frac{v'}{u'}(\epsilon Y - \tilde{a}_1) - \frac{v'}{u'}(-\tilde{a}_1) \right| \geq C_1 \epsilon Y. \quad (83)$$

Thus, there exists  $C_2 > 0$  such that,

$$Y \leq \frac{\alpha \sqrt{3}}{C_1} e^{-2(-\frac{3}{4} \ln(\epsilon))^{\frac{1}{3}} \epsilon Y} e^{\frac{1}{2}(-\frac{3}{4} \ln(\epsilon))^{-\frac{1}{3}} (\epsilon Y)^2} \left( 1 + C_2 \left( \frac{1}{|\ln(\epsilon)|} \right) \right),$$

which rewrites

$$Y e^{2(-\frac{3}{4} \ln(\epsilon))^{\frac{1}{3}} \epsilon Y} \leq \frac{\alpha \sqrt{3}}{C_1} e^{\frac{1}{2}(-\frac{3}{4} \ln(\epsilon))^{-\frac{1}{3}} (\epsilon Y)^2} \left( 1 + C_2 \left( \frac{1}{|\ln(\epsilon)|} \right) \right).$$

But,  $\epsilon Y = X \in [0, \tilde{a}_1)$  is bounded and thus the right member of the previous inequality is bounded by a constant independent of  $\epsilon$  and  $Y$ . Thus, there exists  $C > 0$  such that

$$Y e^{2(-\frac{3}{4} \ln(\epsilon))^{\frac{1}{3}} \epsilon Y} \leq C \quad (84)$$

and

$$\epsilon \left( -\frac{3}{4} \ln(\epsilon) \right)^{\frac{1}{3}} Y e^{2(-\frac{3}{4} \ln(\epsilon))^{\frac{1}{3}} \epsilon Y} \leq \epsilon \left( -\frac{3}{4} \ln(\epsilon) \right)^{\frac{1}{3}} C.$$

The function  $x \mapsto x e^{2x}$  is of class  $C^1$  and strictly increasing on  $\mathbb{R}$ , let us denote by  $h$  its reciprocal function which is also  $C^1$ . From (84) one gets

$$\epsilon \left( -\frac{3}{4} \ln(\epsilon) \right)^{\frac{1}{3}} Y \leq h \left( \epsilon \left( -\frac{3}{4} \ln(\epsilon) \right)^{\frac{1}{3}} C \right).$$

Since  $h$  is of class  $C^1$ ,  $h(0) = 0$ ,  $h'(0) = 1$  and  $\epsilon \left( -\frac{3}{4} \ln(\epsilon) \right)^{\frac{1}{3}} \xrightarrow{\epsilon \rightarrow 0} 0$ , there exists  $D > 0$  such that

$$h \left( \epsilon \left( -\frac{3}{4} \ln(\epsilon) \right)^{\frac{1}{3}} C \right) \leq \epsilon \left( -\frac{3}{4} \ln(\epsilon) \right)^{\frac{1}{3}} C + D \epsilon^2 \left( -\frac{3}{4} \ln(\epsilon) \right)^{\frac{2}{3}}$$



and

$$Y \leq C + D\epsilon \left(-\frac{3}{4} \ln(\epsilon)\right)^{\frac{1}{3}}, \quad (85)$$

from which we deduce that  $Y$  is bounded. Thus,  $X = \mathcal{O}(\epsilon)$ , namely

$$X = \mathcal{O}\left(e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_1)^{\frac{3}{2}}}\right)$$

and since  $X = -\theta E_{\min}^0 - \theta V_0 + \tilde{a}_1$ , we already have

$$\theta E_{\min}^0 = -\theta V_0 + \tilde{a}_1 + \mathcal{O}\left(e^{-\frac{4}{3}(-\tilde{a}_1 + \theta V_0)^{\frac{3}{2}}}\right).$$

We can refine the estimate. Since  $Y$  is bounded,  $\epsilon Y$  tends to 0 and one has

$$\frac{v'}{u'}(\epsilon Y - \tilde{a}_1) - \frac{v'}{u'}(-\tilde{a}_1) = \left(\frac{v'}{u'}\right)'(-\tilde{a}_1)(\epsilon Y) + \mathcal{O}(\epsilon^2).$$

Using (85) to prove that

$$e^{-2\left(-\frac{3}{4} \ln(\epsilon)\right)^{\frac{1}{3}} \epsilon Y} e^{\frac{1}{2}\left(-\frac{3}{4} \ln(\epsilon)\right)^{-\frac{1}{3}} (\epsilon Y)^2} = 1 + \mathcal{O}\left(\epsilon |\ln(\epsilon)|^{\frac{1}{3}}\right),$$

one deduces from (82) that

$$\left(\frac{v'}{u'}\right)'(-\tilde{a}_1) \cdot Y + \mathcal{O}(\epsilon) = \alpha\sqrt{3} \left(1 + \mathcal{O}\left(\frac{1}{|\ln(\epsilon)|}\right) + \mathcal{O}\left(\epsilon |\ln(\epsilon)|^{\frac{1}{3}}\right)\right)$$

hence

$$\left(\frac{v'}{u'}\right)'(-\tilde{a}_1) \cdot Y = \alpha\sqrt{3} \left(1 + \mathcal{O}\left(\frac{1}{|\ln(\epsilon)|}\right)\right).$$

Since  $\left(\frac{v'}{u'}\right)'(-\tilde{a}_1) = \frac{\tilde{a}_1}{(u'(-\tilde{a}_1))^2}$ , when  $\theta V_0$  tends to  $+\infty$  and thus  $\epsilon = e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_1)^{\frac{3}{2}}}$  tends to 0,

$$Y = \alpha\sqrt{3} \frac{(u'(-\tilde{a}_1))^2}{\tilde{a}_1} + \mathcal{O}\left((\theta V_0 - \tilde{a}_1)^{-\frac{3}{2}}\right). \quad (86)$$

Thus,

$$X = \epsilon Y = \alpha\sqrt{3} \frac{(u'(-\tilde{a}_1))^2}{\tilde{a}_1} e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_1)^{\frac{3}{2}}} + \mathcal{O}\left((\theta V_0 - \tilde{a}_1)^{-\frac{3}{2}} e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_1)^{\frac{3}{2}}}\right)$$

and finally, using  $\theta E_{\min}^0 = -X - \theta V_0 + \tilde{a}_1$

$$\theta E_{\min}^0 = -\theta V_0 + \tilde{a}_1 - \alpha\sqrt{3} \frac{(u'(-\tilde{a}_1))^2}{\tilde{a}_1} e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_1)^{\frac{3}{2}}} + \mathcal{O}\left((\theta V_0 - \tilde{a}_1)^{-\frac{3}{2}} e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_1)^{\frac{3}{2}}}\right),$$

which proves the second point. This is an estimate in the semiclassical limit.

**(3)** For the last point, we look at the behaviour of  $\theta E_{\min}^0$  when  $\theta V_0$  tends to 0. Since  $E_{\min}^0$  is a solution of (66) with  $-\theta E_{\min}^0 > 0$  and  $-\theta V_0 - \theta E_{\min}^0 \in (-\tilde{a}_1, 0)$ , when  $\theta V_0$  tends to 0, both  $-\theta E_{\min}^0$  and  $-\theta V_0 - \theta E_{\min}^0$  tends to 0. In order to avoid the technical difficulty induced by the fact that  $\frac{v'}{u'}$  tends to  $+\infty$  at 0, we use the fact that  $E_{\min}^0$  is also the unique solution in  $(-V_0, 0)$  of the equation

$$\frac{u'}{v'}(-\theta V_0 - \theta E) = \frac{u'}{v'}(-\theta E). \quad (87)$$

Note that  $u$  and  $v$  stand for  $f$  and  $g$  in [1, 10.4.3]. Thus, for  $x$  in a neighborhood of 0 where  $v'$  does not vanish,

$$\left(\frac{u'}{v'}\right)'(x) = \frac{x}{(v'(x))^2} \quad \text{and} \quad v(x) = x + \frac{x^4}{12} + \mathcal{O}(x^7).$$

One deduces

$$\left(\frac{u'}{v'}\right)'(x) = x - \frac{2}{3}x^4 + \mathcal{O}(x^7)$$

hence

$$\left(\frac{u'}{v'}\right)'(x) = \left(\frac{u'}{v'}\right)'(0) + \frac{1}{2}x^2 - \frac{2}{15}x^5 + \mathcal{O}(x^8). \quad (88)$$

Let  $y = -\theta E_{\min}^0 - \frac{\theta V_0}{2}$ . Then, (87) rewrites

$$\frac{u'}{v'}\left(y - \frac{\theta V_0}{2}\right) = \frac{u'}{v'}\left(y + \frac{\theta V_0}{2}\right). \quad (89)$$

Since  $-\theta V_0 < \theta E_{\min}^0 < 0$ ,

$$|y| \leq \frac{\theta V_0}{2}. \quad (90)$$

By (90),  $y = \mathcal{O}(\theta V_0)$ . Thus equation (89) and equality (88) imply

$$\begin{aligned} \frac{1}{2} \left( y^2 + \left(\frac{\theta V_0}{2}\right)^2 - \theta V_0 y \right) - \frac{2}{15} \left( y - \frac{\theta V_0}{2} \right)^5 = \\ \frac{1}{2} \left( y^2 + \left(\frac{\theta V_0}{2}\right)^2 + \theta V_0 y \right) - \frac{2}{15} \left( y + \frac{\theta V_0}{2} \right)^5 + \mathcal{O}((\theta V_0)^8) \end{aligned}$$

that is

$$-\theta V_0 y - \frac{2}{15} \left( -5\theta V_0 y^4 - 20 \left(\frac{\theta V_0}{2}\right)^3 y^2 - 2 \left(\frac{\theta V_0}{2}\right)^5 \right) + \mathcal{O}((\theta V_0)^8) = 0,$$

which implies

$$y - \frac{2}{15}y^4 - \frac{4}{3} \left(\frac{\theta V_0}{2}\right)^3 y^2 = \frac{2}{15} \left(\frac{\theta V_0}{2}\right)^4 + \mathcal{O}((\theta V_0)^7). \quad (91)$$

Then, (90) and (91) give  $y = \mathcal{O}((\theta V_0)^4)$ . We write  $y = (\theta V_0)^4 \rho$  where  $\rho$  is a bounded function of  $\theta V_0$ . Then, (91) rewrites

$$\rho - \frac{2}{15}(\theta V_0)^{12} \rho^4 = \frac{1}{120} + \mathcal{O}((\theta V_0)^3),$$

hence

$$\rho = \frac{1}{120} + \mathcal{O}((\theta V_0)^3)$$

and then,

$$y = \frac{1}{120}(\theta V_0)^4 + \mathcal{O}((\theta V_0)^7),$$

which proves (10). □

To finish this Section and before turning to the study of the upper edge of the first spectral band, we prove Proposition 1.

*Proof:* Let  $(e_1, \dots, e_d)$  be the canonical basis of  $\mathbb{R}^d$  and  $F_{d-1} = \text{Vect}(e_2, \dots, e_d)$ . Since  $V_d$  is a potential which has separable variables, we have a tensor product decomposition for  $H_d$ :

$$H_d = \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V \right) \otimes \text{Id}_{(x_2, \dots, x_d)} + \text{Id}_{x_1} \otimes \left( -\frac{\hbar^2}{2m} \Delta_{d-1} \right)$$

where  $\text{Id}_{(x_2, \dots, x_d)}$  is the identity operator on  $F_{d-1}$ ,  $\text{Id}_{x_1}$  is the identity on  $\text{Vect}(e_1)$  and  $\Delta_{d-1}$  is the Laplacian acting on  $H^2(F_{d-1})$ .

Then, using general results on the spectrum of tensor products of operators (see [25, Theorem VIII.33]), we obtain:

$$\begin{aligned} \sigma(H_d) &= \sigma \left( \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V \right) \otimes \text{Id}_{(x_2, \dots, x_d)} \right) + \sigma \left( \text{Id}_{x_1} \otimes \left( -\frac{\hbar^2}{2m} \Delta_{d-1} \right) \right) \\ &= \sigma(H) + \sigma(-\Delta_{d-1}) \\ &= \bigcup_{p \geq 0} [E_{\min}^p, E_{\max}^p] + [0, +\infty) \\ &= [E_{\min}^0, +\infty). \end{aligned}$$

Since  $H$  has purely absolutely continuous spectrum and  $-\frac{\hbar^2}{2m} \Delta_{d-1}$  too, the spectrum of  $H_d$  is also purely absolutely continuous.  $\square$

**6.3. The upper edge of the first spectral band.** The upper edge of the first spectral band is the smallest value of  $E$  among the solutions of equations (68) and (69).

We start by assuming that  $\theta V_0 \in [c_0, \tilde{c}_0)$ , which implies in particular that we are in the semiclassical regime. In this case (69) has no solution with  $-\theta E > 0$  and we prove that (68) has a unique solution such that  $-\theta E > 0$  and  $-\theta V_0 - \theta E \in [-c_0, -\tilde{a}_1)$ . Indeed, the function  $z_0 : [0, +\infty) \rightarrow [c_0, +\infty)$  is a continuous bijection and

$$\forall \theta V_0 \geq c_0, \exists! x_0 \geq 0, z_0(x_0) = x_0 - \psi_0(x_0) = \theta V_0.$$

One sets  $\check{E}_0 = -\frac{x_0}{\theta}$  and since  $x_0 = \theta V_0 + \psi_0(x_0) \in [-c_0 + \theta V_0, -\tilde{a}_1 + \theta V_0)$  one has

$$-V_0 + \frac{\tilde{a}_1}{\theta} < \check{E}_0 \leq -V_0 + \frac{c_0}{\theta}.$$

Thus, for  $\theta V_0 \in [c_0, \tilde{c}_0)$ ,  $E_{\max}^0 = \check{E}_0$ .

We then assume that  $\theta V_0 \geq \tilde{c}_0$ . In this case, (68) has still a unique solution such that  $-\theta E > 0$  and  $-\theta V_0 - \theta E \in [-c_0, -\tilde{a}_1)$ , namely  $\check{E}_0$ , but one can also find a solution of (69) with  $-\theta E > 0$ . Indeed, the function from  $[0, +\infty) \rightarrow [\tilde{c}_0, +\infty)$  which maps  $x \geq 0$  to  $x - \psi^0(x)$  is a continuous strictly increasing bijection. Thus,

$$\forall \theta V_0 \geq \tilde{c}_0, \exists! \tilde{x}_0 \geq 0, \tilde{x}_0 - \psi^0(\tilde{x}_0) = \theta V_0.$$

One sets  $\tilde{E}_0 = -\frac{\tilde{x}_0}{\theta}$  and since  $\tilde{x}_0 = \theta V_0 + \psi^0(\tilde{x}_0) \in (-a_1 + \theta V_0, -\tilde{c}_0 + \theta V_0]$  one has

$$-V_0 + \frac{\tilde{c}_0}{\theta} \leq \tilde{E}_0 < -V_0 + \frac{a_1}{\theta}.$$

Since  $c_0 < \tilde{c}_0$ , one has  $\check{E}_0 < \tilde{E}_0$  which implies  $E_{\max}^0 = \check{E}_0$  and  $E_{\min}^1 = \tilde{E}_0$ .

As we identified  $E_{\max}^0$  among all the solutions of (68) and (69), we can give more precise estimates.

**Proposition 6.** *We have the following estimates on  $E_{\max}^0$ , in the semiclassical regime and the semiclassical limit:*

(1) For every  $\theta V_0 > c_0$ ,

$$-V_0 + \frac{\tilde{a}_1}{\theta} < E_{\max}^0 < -V_0 + \frac{c_0}{\theta}.$$

(2) When  $\theta V_0$  tends to  $+\infty$ ,

$$\theta E_{\max}^0 = -\theta V_0 + \tilde{a}_1 + \alpha \sqrt{3} \frac{(u'(-\tilde{a}_1))^2}{\tilde{a}_1} e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_1)^{\frac{3}{2}}} \left(1 + \mathcal{O}\left((\theta V_0 - \tilde{a}_1)^{-\frac{3}{2}}\right)\right).$$

*Proof:* (1) The first point has just been proven before we stated Proposition 6 and the strict inequality is a consequence of the strictly increasing character of  $z_0$ .

(2) For the second point, we follow the proof of point 3 of Theorem 3. We assume that  $\theta V_0 > \tilde{a}_1$ . One sets  $X = -\theta E_{\max}^0 - \theta V_0 + \tilde{a}_1$ , then  $X$  satisfies

$$\frac{v'}{u'}(X - \tilde{a}_1) = \frac{v}{u}(X + \theta V_0 - \tilde{a}_1), \quad X \in [-c_0 + \tilde{a}_1, 0]. \quad (92)$$

Using [1, 10.4.59, 10.4.63] in the equality (78), one gets

$$\frac{v'}{u'}(X - \tilde{a}_1) = \alpha - \alpha \sqrt{3} e^{-\frac{4}{3}(X + \theta V_0 - \tilde{a}_1)^{\frac{3}{2}}} \left(1 + \mathcal{O}\left((X + \theta V_0 - \tilde{a}_1)^{-\frac{3}{2}}\right)\right). \quad (93)$$

Again, we set  $\epsilon = e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_1)^{\frac{3}{2}}}$ . We also define  $Y$  as in the proof of point (3) of Theorem 3. Then, equality (81) is still valid and the condition  $X \in [-c_0 + \tilde{a}_1, 0]$  implies that

$$-c_0 + \tilde{a}_1 + \left(-\frac{3}{4} \ln(\epsilon)\right)^{\frac{2}{3}} = -c_0 + \theta V_0 \leq X + \theta V_0 - \tilde{a}_1 \leq \left(-\frac{3}{4} \ln(\epsilon)\right)^{\frac{2}{3}}$$

and in particular,  $X + \theta V_0 - \tilde{a}_1$  tends to  $+\infty$  when  $\theta V_0$  tends to  $+\infty$ . Moreover,

$$\frac{4}{3} \frac{1}{|\ln(\epsilon)|} \leq (X + \theta V_0 - \tilde{a}_1)^{-\frac{3}{2}} \leq \left(\left(\frac{3}{4}\right)^{\frac{2}{3}} + \frac{\tilde{a}_1 - c_0}{|\ln(\epsilon)|^{\frac{2}{3}}}\right)^{-\frac{3}{2}} \frac{1}{|\ln(\epsilon)|}.$$

Using (93) and the relation  $\alpha = \frac{v'}{u'}(-\tilde{a}_1)$  one gets:

$$\begin{aligned} \frac{1}{\epsilon} \left( \frac{v'}{u'}(\epsilon Y - \tilde{a}_1) - \frac{v'}{u'}(-\tilde{a}_1) \right) = \\ -\alpha \sqrt{3} e^{-2\left(-\frac{3}{4} \ln(\epsilon)\right)^{\frac{1}{3}} \epsilon Y} e^{-\frac{1}{3}\left(-\frac{3}{4} \ln(\epsilon)\right)^2 (\epsilon Y)^2 Q(\epsilon Y)} \left(1 + \mathcal{O}\left(\frac{1}{|\ln(\epsilon)|}\right)\right). \end{aligned} \quad (94)$$

Inequality (83) is still valid and, using the fact that  $\epsilon Y = X \in [-c_0 - \tilde{a}_1, 0]$ , one gets that  $Y$  is bounded and

$$X = \mathcal{O}\left(e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_1)^{\frac{3}{2}}}\right).$$

Then, the bootstrap argument gives us the limit of  $Y$  and we have

$$Y = -\alpha \sqrt{3} \frac{(u'(-\tilde{a}_1))^2}{\tilde{a}_1} + \mathcal{O}\left((\theta V_0 - \tilde{a}_1)^{-\frac{3}{2}}\right)$$

and

$$\theta E_{\max}^0 = -\theta V_0 + \tilde{a}_1 + \alpha \sqrt{3} \frac{(u'(-\tilde{a}_1))^2}{\tilde{a}_1} e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_1)^{\frac{3}{2}}} + \mathcal{O}\left((\theta V_0 - \tilde{a}_1)^{-\frac{3}{2}} e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_1)^{\frac{3}{2}}}\right),$$

which proves the second point.  $\square$

We deduce from the asymptotic expansions in  $\theta V_0$  of  $E_{\min}^0$  and  $E_{\max}^0$  the width of the first rescaled spectral band in the semiclassical limit.

**Proposition 7.** *When  $\theta V_0$  tends to  $+\infty$ ,*

$$\theta E_{\max}^0 - \theta E_{\min}^0 = 2\alpha \sqrt{3} \frac{(u'(-\tilde{a}_1))^2}{\tilde{a}_1} e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_1)^{\frac{3}{2}}} \left(1 + \mathcal{O}\left((\theta V_0 - \tilde{a}_1)^{-\frac{3}{2}}\right)\right). \quad (95)$$

For  $\theta V_0 \leq c_0$  (*i.e.* in the classical regime), the situation changes. The first band recovers completely the range of the periodic potential  $V$  and is even larger.

**Proposition 8.** *If  $\theta V_0 \leq c_0$ ,  $E_{\max}^0 \geq 0$  and we have*

$$\left[\min\left(-\frac{V_0}{2}, -V_0 + \frac{\tilde{a}_1}{\theta}\right), 0\right] \subset [E_{\min}^0, E_{\max}^0].$$

*Proof:* If  $\theta V_0 \leq c_0$ , there is no longer a solution of (68) or (69) satisfying  $-\theta E > 0$ . Thus,  $-\theta E \leq 0$  and  $E_{\max}^0 \geq 0$ . Using the upper bound on  $E_{\min}^0$  given in Theorem 3, we have  $-V_0 + \frac{\tilde{a}_1}{\theta} \in [E_{\min}^0, E_{\max}^0]$ . Using point (1) of Theorem 3, we also have  $-\frac{V_0}{2} \in [E_{\min}^0, E_{\max}^0]$ , which proves the proposition.  $\square$

Proposition 8 along with Proposition 6 imply Theorem 1.

The following proposition precise the behaviour of  $E_{\max}^0$  in the classical regime and the classical limit.

**Proposition 9.** *Let  $\theta V_0 \leq c_0$ .*

- (1) *If  $\theta V_0 \in (\tilde{c}_1 - \tilde{c}_0, c_0]$ , then  $\theta E_{\max}^0 \in (-\theta V_0 + \tilde{c}_0, 0]$ .*
- (2) *If  $\theta V_0 < \tilde{c}_1 - \tilde{c}_0$ , let  $p_0$  defined in (7). Then,  $\theta E_{\max}^0 \in [-\theta V_0 + \tilde{c}_{p_0}, \tilde{c}_{p_0+1}]$  or  $\theta E_{\max}^0 \in [-\theta V_0 + \tilde{c}_{p_0-1}, \tilde{c}_{p_0}]$ .*
- (3)

$$\lim_{\theta V_0 \rightarrow 0} \theta E_{\max}^0 = +\infty. \quad (96)$$

*Proof:* **(2)** Since  $(\tilde{c}_{k+1} - \tilde{c}_k)_{k \geq 0}$  is strictly decreasing and converges to 0, for any  $\theta V_0 \in [0, \tilde{c}_1 - \tilde{c}_0)$ , the integer  $p_0 \geq 1$  defined in (7) is well defined and unique.

$E_{\max}^0$  is a solution of either (69) or (68). Let  $k \geq 1$ . The restriction of the function  $\frac{v}{u}$  to  $(-\tilde{c}_{2k}, -\tilde{c}_{2k-2})$  is a strictly increasing and continuous bijection from  $(-\tilde{c}_{2k}, -\tilde{c}_{2k-2})$  to  $\mathbb{R}$  denoted by  $\left(\frac{v}{u}\right)_{2k-2}$ , and  $\frac{v'}{u'}$  induce a strictly increasing and continuous bijection from  $(-\tilde{c}_{2k+1}, -\tilde{c}_{2k-1})$  to  $\mathbb{R}$  denoted by  $\left(\frac{v'}{u'}\right)_{2k-1}$ . Then, studying the sign of  $f_x$  for  $x \in (-\tilde{c}_{2k}, -\tilde{c}_{2k-2})$  and using the Sturm-Picone's lemma in a way similar as in the proof of Lemma 10, we prove that  $x \mapsto x - \left(\frac{v'}{u'}\right)_{2k-1}^{-1} \left(\frac{v}{u}\right)_{2k-2}(x)$  is strictly increasing and continuous from  $(-\tilde{c}_{2k+1}, -\tilde{c}_{2k-1})$  to  $(\tilde{c}_{2k+1} - \tilde{c}_{2k}, \tilde{c}_{2k-1} - \tilde{c}_{2k-2})$ .

Thus, (68) admits a unique solution  $\underline{E}_k$  with  $-\theta\underline{E}_k \in (-\tilde{c}_{2k}, -\tilde{c}_{2k-2})$  and  $-\theta V_0 - \theta\underline{E}_k \in (-\tilde{c}_{2k+1}, -\tilde{c}_{2k-1})$ .

To study the sign of  $f_x$ , we need to know the signs of  $u$ ,  $v$ ,  $u'$  and  $v'$  on the interval  $(-\tilde{c}_{2k+1}, -\tilde{c}_{2k-2})$ , since  $x \in (-\tilde{c}_{2k}, -\tilde{c}_{2k-2})$  and  $x - z \in (-\tilde{c}_{2k+1}, -\tilde{c}_{2k-1})$ . For example, we have on  $(-\tilde{c}_{2k+1}, -c_{2k+1})$ ,

$$(-1)^k u < 0, \quad (-1)^k u' > 0, \quad (-1)^k v > 0, \quad (-1)^k v' < 0$$

and on  $(-c_{2k+1}, -\tilde{c}_{2k})$ ,

$$(-1)^k u < 0, \quad (-1)^k u' > 0, \quad (-1)^k v < 0, \quad (-1)^k v' < 0$$

and the signs alternate on the successive intervals  $(-\tilde{c}_{2k}, -c_{2k})$ ,  $(-c_{2k}, -\tilde{c}_{2k-1})$ ,  $(-\tilde{c}_{2k-1}, -c_{2k-1})$ ,  $(-c_{2k-1}, -\tilde{c}_{2k-2})$ .

The restriction of the function  $\frac{v}{u}$  to  $(-\tilde{c}_{2k+2}, -\tilde{c}_{2k})$  is a strictly increasing and continuous bijection from  $(-\tilde{c}_{2k+2}, -\tilde{c}_{2k})$  to  $\mathbb{R}$  denoted by  $\left(\frac{v}{u}\right)_{2k}$ . We set for every  $x \in (-\tilde{c}_{2k+1}, -\tilde{c}_{2k-1})$  and every  $z \in (-\tilde{c}_{2k+1} + \tilde{c}_{2k+2}, -\tilde{c}_{2k-1} + \tilde{c}_{2k})$ ,  $\bar{g}_x(z) = v(x - z)u'(x) - u(x - z)v'(x)$ . Then  $\bar{g}_x$  satisfies the Airy equation and using the signs of  $u$ ,  $v$ ,  $u'$  and  $v'$  given above and a Sturm-Picone's argument as in Lemma 10, we prove that  $x \mapsto x - \left(\frac{v}{u}\right)_{2k}^{-1} \left(\frac{v'}{u'}\right)_{2k-1}(x)$  is strictly increasing and continuous from  $(-\tilde{c}_{2k+1}, -\tilde{c}_{2k-1})$  to  $(-\tilde{c}_{2k+1} + \tilde{c}_{2k+2}, -\tilde{c}_{2k-1} + \tilde{c}_{2k})$ .

Thus, (69) admits a unique solution  $\bar{E}_k$  with  $-\theta\bar{E}_k \in (-\tilde{c}_{2k+1}, -\tilde{c}_{2k-1})$  and  $-\theta V_0 - \theta\bar{E}_k \in (-\tilde{c}_{2k+2}, -\tilde{c}_{2k})$ .

Since  $\tilde{c}_{p_0+1} - \tilde{c}_{p_0} < \theta V_0 < \tilde{c}_{p_0} - \tilde{c}_{p_0-1}$ , we have either  $E_{\max}^0 = \underline{E}_k$  or  $E_{\max}^0 = \bar{E}_k$  for  $k$  equal to the integer part of  $\frac{p_0}{2}$ .

We deduce that  $-\theta E_{\max}^0 \in [-\tilde{c}_{p_0+1}, -\tilde{c}_{p_0-1}]$  and  $-\theta V_0 - \theta E_{\max}^0 \in [-\tilde{c}_{p_0+2}, -\tilde{c}_{p_0}]$ , or  $-\theta E_{\max}^0 \in [-\tilde{c}_{p_0}, -\tilde{c}_{p_0-2}]$  and  $-\theta V_0 - \theta E_{\max}^0 \in [-\tilde{c}_{p_0+1}, -\tilde{c}_{p_0-1}]$ . This proves the second point.

**(1)** If  $\theta V_0 \in (\tilde{c}_1 - \tilde{c}_0, c_0]$ , then  $\theta V_0 \in (\tilde{c}_2 - \tilde{c}_1, \tilde{c}_0)$ . The function  $\frac{v'}{u'}$  induces a strictly increasing and continuous bijection from  $(-\tilde{c}_1, 0)$  to  $\mathbb{R}$  denoted by  $\left(\frac{v'}{u'}\right)_0$ .

Then, with the previous notations, the function  $x \mapsto x - \left(\frac{v}{u}\right)_0^{-1} \left(\frac{v'}{u'}\right)_0(x)$  is strictly increasing and continuous from  $(-\tilde{c}_1, 0)$  to  $(\tilde{c}_2 - \tilde{c}_1, \tilde{c}_0)$ , using again Sturm-Picone's Lemma with  $\bar{g}_x$  for  $x \in (-\tilde{c}_1, 0)$ . Thus, (69) admits a unique solution  $\bar{E}_0$  with  $-\theta\bar{E}_0 \in (-\tilde{c}_1, 0)$  and  $-\theta V_0 - \theta\bar{E}_0 \in (-\tilde{c}_2, -\tilde{c}_0)$ . Since  $E_{\max}^0 = \bar{E}_0$ , we proved the first point.

**(3)** The integer  $p_0$  tends to  $+\infty$  when  $\theta V_0$  tends to 0. Indeed, using (54) and (56), one has

$$p_0 = \mathcal{O}((\theta V_0)^{-3}).$$

Since  $p_0 \xrightarrow{\theta V_0 \rightarrow 0} +\infty$  and  $c_k \xrightarrow{k \rightarrow +\infty} +\infty$ , we get (96) and prove the third point.  $\square$

Proposition 9 and Theorem 3 imply directly Theorem 2.

**6.4. The first spectral gap.** In the discussion before the statement of Proposition 6, we identified both  $E_{\max}^0$  and  $E_{\min}^1$  in the case  $\theta V_0 \geq \tilde{c}_0$ . We had obtained, for every  $\theta V_0 \geq \tilde{c}_0$ ,

$$-V_0 + \frac{\tilde{a}_1}{\theta} < E_{\max}^0 \leq -V_0 + \frac{c_0}{\theta}$$

and

$$-V_0 + \frac{\tilde{c}_0}{\theta} \leq E_{\min}^1 < -V_0 + \frac{a_1}{\theta}.$$

This yields a first estimate of the first spectral gap in the semiclassical regime

$$0 < \frac{\tilde{c}_0 - c_0}{\theta} \leq E_{\min}^1 - E_{\max}^0 < \frac{a_1 - \tilde{a}_1}{\theta}.$$

In particular, the first gap is always open.

Similarly to the expansions we obtained for the edges of the first spectral band, we can prove the following expansion for  $\theta E_{\min}^1$  in the semiclassical limit.

**Proposition 10.** *When  $\theta V_0$  tends to  $+\infty$ ,*

$$\theta E_{\min}^1 = -\theta V_0 + a_1 - \alpha \sqrt{3} (u(-a_1))^2 e^{-\frac{4}{3}(\theta V_0 - a_1)^{\frac{3}{2}}} \left( 1 + \mathcal{O} \left( (\theta V_0 - a_1)^{-\frac{3}{2}} \right) \right). \quad (97)$$

*Proof:* We follow the proof of point 3 of Theorem 3. We assume that  $\theta V_0 > a_1$ . One sets  $X = -\theta E_{\min}^1 - \theta V_0 + a_1$  which satisfies

$$\frac{v}{u}(X - a_1) = \frac{v'}{u'}(X + \theta V_0 - a_1), \quad X \in [0, -\tilde{c}_0 + a_1]. \quad (98)$$

Since  $x \mapsto x - \psi^0$  is strictly increasing on  $[0, +\infty)$ , there exists  $C > 0$  such that for  $\theta V_0 > C$ ,  $-\theta E_{\min}^1 - \theta V_0 \in [-a_1, \frac{-\tilde{c}_0 - a_1}{2}]$  and thus  $X \in [0, \frac{-\tilde{c}_0 + a_1}{2}]$ .

Using [1, 10.4.61, 10.4.66] in the equality (78), one gets

$$\frac{v}{u}(X - a_1) = \alpha + \alpha \sqrt{3} e^{-\frac{4}{3}(X + \theta V_0 - a_1)^{\frac{3}{2}}} \left( 1 + \mathcal{O} \left( (X + \theta V_0 - a_1)^{-\frac{3}{2}} \right) \right). \quad (99)$$

We set  $\epsilon = e^{-\frac{4}{3}(\theta V_0 - a_1)^{\frac{3}{2}}}$  and  $Y = \frac{1}{\epsilon} X$ . Since  $\alpha = \frac{v}{u}(-a_1)$  and using the fact that  $\left(\frac{v}{u}\right)' = \frac{1}{u^2}$  is bounded from below by a strictly positive constant on  $[0, \frac{-\tilde{c}_0 + a_1}{2}]$ , one shows with a similar proof as (83) that:

$$\exists C_2 > 0, \quad \left| \frac{v}{u}(X - a_1) - \frac{v}{u}(-a_1) \right| \geq C_2 \epsilon Y.$$

Then, following the proof of point 3 of Theorem 3 and using that  $\epsilon Y = X \in [0, \frac{-\tilde{c}_0 + a_1}{2}]$  is bounded, one gets that  $Y$  is bounded and

$$X = \mathcal{O} \left( e^{-\frac{4}{3}(\theta V_0 - a_1)^{\frac{3}{2}}} \right).$$

Since  $Y$  is bounded one has:

$$\frac{v}{u}(\epsilon Y - a_1) - \frac{v}{u}(-a_1) = \left(\frac{v}{u}\right)'(-a_1)(\epsilon Y) + \mathcal{O}(\epsilon^2).$$

But,  $\left(\frac{v}{u}\right)'(-a_1) = \frac{1}{(u(-a_1))^2}$  and we get, similarly to (86),

$$Y = \alpha \sqrt{3} (u(-a_1))^2 + \mathcal{O} \left( (\theta V_0 - a_1)^{-\frac{3}{2}} \right)$$

from which we obtain (97). □

Combining the asymptotics of  $\theta E_{\max}^0$  and  $\theta E_{\min}^1$  we deduce an asymptotic expansion of the rescaled first gap in the semiclassical limit.

**Proposition 11.** *When  $\theta V_0$  tends to  $+\infty$ ,*

$$\theta E_{\min}^1 - \theta E_{\max}^0 = a_1 - \tilde{a}_1 - \alpha\sqrt{3}(u(-a_1))^2 e^{-\frac{4}{3}(\theta V_0 - a_1)^{\frac{3}{2}}} \left(1 + \mathcal{O}\left((\theta V_0 - a_1)^{-\frac{3}{2}}\right)\right). \quad (100)$$

*Proof:* We combine (97) and point (2) of Proposition 6. Then, since  $a_1 > \tilde{a}_1$ , one has

$$(\theta V_0 - \tilde{a}_1)^{-\frac{3}{2}} e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_1)^{\frac{3}{2}}} \leq (\theta V_0 - a_1)^{-\frac{3}{2}} e^{-\frac{4}{3}(\theta V_0 - a_1)^{\frac{3}{2}}},$$

which allows to keep only the term  $\mathcal{O}\left((\theta V_0 - a_1)^{-\frac{3}{2}} e^{-\frac{4}{3}(\theta V_0 - a_1)^{\frac{3}{2}}}\right)$  and not the term  $\mathcal{O}\left((\theta V_0 - \tilde{a}_1)^{-\frac{3}{2}} e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_1)^{\frac{3}{2}}}\right)$  in (100).  $\square$

## 7. THE $p$ FIRST SPECTRAL BANDS IN THE SEMICLASSICAL REGIME

In this Section, we prove Theorem 4 by determining the band edges which are contained in the interval  $[-V_0, 0]$  for a fixed  $\theta V_0$ .

**Proposition 12.** *Let  $p \geq 0$  and assume that  $\theta V_0 \geq \tilde{c}_p$ . Then, for every  $k \in \{0, \dots, p\}$ ,*

- (1) *If  $k = 2j$  is even, (69) has a unique solution  $\hat{E}_{2j}$  with  $-\theta E \in [0, +\infty)$ ,  $-\theta V_0 - \theta E \in (-a_{j+1}, -\tilde{c}_{2j}]$  and satisfying:*

$$-V_0 + \frac{\tilde{c}_{2j}}{\theta} \leq \hat{E}_{2j} < -V_0 + \frac{a_{j+1}}{\theta}. \quad (101)$$

- (2) *If  $k = 2j + 1$  is odd, (66) has a unique solution  $\hat{E}_{2j+1}$  with  $-\theta E \in [0, +\infty)$ ,  $-\theta V_0 - \theta E \in (-\tilde{a}_{j+2}, -\tilde{c}_{2j+1}]$  and satisfying:*

$$-V_0 + \frac{\tilde{c}_{2j+1}}{\theta} \leq \hat{E}_{2j+1} < -V_0 + \frac{\tilde{a}_{j+2}}{\theta}. \quad (102)$$

*Proof:* By Lemma 5, for every  $k \geq 0$ , the function  $x \mapsto x - \psi^k(x)$  is a strictly increasing and continuous bijection from  $[0, +\infty)$  to  $[\tilde{c}_k, +\infty)$ . Thus, if  $\theta V_0 \geq \tilde{c}_p \geq \tilde{c}_k$ , there exists a unique  $x^k \geq 0$  such that  $\theta V_0 = x^k - \psi^k(x^k)$ . Let  $\hat{E}_k$  be such that  $-\theta \hat{E}_k = x^k$ . Then, if  $k = 2j$ ,  $\hat{E}_{2j}$  is the unique solution of (69) with  $-\theta E \in [0, +\infty)$  and  $-\theta V_0 - \theta E \in (-a_{j+1}, -\tilde{c}_{2j}]$ . Moreover,

$$-a_{j+1} < -\theta \hat{E}_k - \theta V_0 \leq -\tilde{c}_k < 0 \leq -\theta \hat{E}_k,$$

and we get (101). If  $k = 2j + 1$ ,  $\hat{E}_{2j+1}$  is the unique solution of (66) with  $-\theta E \in [0, +\infty)$  and  $-\theta V_0 - \theta E \in (-\tilde{a}_{j+2}, -\tilde{c}_{2j+1}]$ . Moreover,

$$-\tilde{a}_{j+2} < -\theta \hat{E}_k - \theta V_0 \leq -\tilde{c}_k < 0 \leq -\theta \hat{E}_k,$$

and we get (102). The proof of the proposition is complete.  $\square$

**Proposition 13.** *Assume that  $\theta V_0 \geq c_p$ . Then, for every  $k \in \{0, \dots, p\}$ ,*

- (1) *If  $k = 2j$  is even, (68) has a unique solution  $\check{E}_{2j}$  with  $-\theta E \in [0, +\infty)$ ,  $-\theta V_0 - \theta E \in [c_{2j}, -\tilde{a}_{j+1}]$  and satisfying:*

$$-V_0 + \frac{\tilde{a}_{j+1}}{\theta} < \check{E}_{2j} \leq -V_0 + \frac{c_{2j}}{\theta}. \quad (103)$$



- (2) If  $k = 2j + 1$  is odd, (67) has a unique solution  $\check{E}_{2j+1}$  with  $-\theta E \in [0, +\infty)$ ,  $-\theta V_0 - \theta E \in [c_{2j+1}, -a_{j+1})$  and satisfying:

$$-V_0 + \frac{a_{j+1}}{\theta} < \check{E}_{2j+1} \leq -V_0 + \frac{c_{2j+1}}{\theta}. \quad (104)$$

*Proof:* Let  $k \in \{0, \dots, p\}$ . Since  $\theta V_0 \geq c_p$ , we have  $\theta V_0 \in [c_k, +\infty)$ . Thanks to Lemma 10,  $z_k$  is continuous and strictly increasing, there exists a unique real number  $x_k \geq 0$  such that  $\theta V_0 = z_k(x_k)$ . Let  $\check{E}_k$  be such that  $-\theta \check{E}_k = x_k$ . Then,  $\check{E}_{2j}$  is the unique solution of (68) such that  $-\theta E \in [0, +\infty)$  and  $-\theta V_0 - \theta E \in [c_{2j}, -\tilde{a}_{j+1})$ . Moreover,

$$-c_k \leq -\theta \check{E}_k - \theta V_0 < -\tilde{a}_{j+1}$$

and we get (103).

Similarly,  $\check{E}_{2j+1}$  is the unique solution of (67) such that  $-\theta E \in [0, +\infty)$  and  $-\theta V_0 - \theta E \in [c_{2j+1}, -a_{j+1})$ . Moreover,

$$-c_k \leq -\theta \check{E}_k - \theta V_0 < -a_{j+1}$$

and we get (104). □

We can deduce from Proposition 12 and Proposition 13 the following Proposition on the  $p$  first spectral bands and the  $p - 1$  first spectral gaps of the operator  $H$ .

**Proposition 14.** *Let  $p \geq 0$ . Assume that  $\theta V_0 \geq \tilde{c}_p$ .*

- (1) For every  $k \in \{0, \dots, p\}$ ,  $E_{\min}^{k+1} = \hat{E}_k$  and  $E_{\max}^k = \check{E}_k$ .  
(2) We have the estimates on the spectral gaps:

$$\forall j \geq 1, 0 < \frac{\tilde{c}_{2j-1} - c_{2j-1}}{\theta} \leq E_{\min}^{2j} - E_{\max}^{2j-1} \leq \frac{\tilde{a}_{j+1} - a_j}{\theta}$$

and

$$\forall j \geq 0, 0 < \frac{\tilde{c}_{2j} - c_{2j}}{\theta} \leq E_{\min}^{2j+1} - E_{\max}^{2j} \leq \frac{a_{j+1} - \tilde{a}_{j+1}}{\theta}.$$

In particular, all the spectral gaps are open.

*Proof:* (1) Using the estimates obtained on  $\hat{E}_k$  and  $\check{E}_k$  and using the fact that  $c_k < \tilde{c}_k$ , we have  $\check{E}_k < \hat{E}_k$ . Since

$$-V_0 < E_{\min}^0 < -V_0 + \frac{\tilde{a}_1}{\theta} < \check{E}_0 < \hat{E}_0,$$

we have  $E_{\max}^0 = \check{E}_0$  and  $E_{\min}^1 = \hat{E}_0$ . Then using  $\check{E}_k < \hat{E}_k$ , we deduce the first point.

(2) These two estimates are deduced directly from the estimates proven on  $\hat{E}_k$  and  $\check{E}_k$  in Proposition 12 and Proposition 13. We just have to be careful with the fact that  $E_{\min}^{2j} = \hat{E}_{2j-1}$  and  $E_{\min}^{2j+1} = \hat{E}_{2j}$  and to use the right estimate in Proposition 12 depending on the parity of  $k$ . □

Propositions 12, 13 and 14 imply the proof of Theorem 5.

*Proof:* (of Theorem 5). For every  $p \geq 0$ ,  $-\theta E_{\max}^p(\theta V_0) = (z_p)^{-1}(\theta V_0)$  and since  $z_p$  is strictly increasing and continuous on  $[0, +\infty)$ ,  $\theta V_0 \mapsto \theta E_{\max}^p(\theta V_0)$  is strictly

decreasing and continuous on  $[0, +\infty)$ . Since for every  $p \geq 0$ ,  $\theta E_{\max}^p(c_p) = 0$ ,  $c_p$  is the unique zero in  $[0, +\infty)$  of the function  $\theta V_0 \mapsto \theta E_{\max}^p(\theta V_0)$ .

Since for every  $p \geq 0$ ,  $-\theta E_{\min}^{p+1}(\theta V_0) = (z^p)^{-1}(\theta V_0)$  (where  $z^p : x \mapsto x - \psi^p(x)$  is strictly increasing and continuous on  $[0, +\infty)$ ),  $\theta V_0 \mapsto \theta E_{\min}^{p+1}(\theta V_0)$  is also strictly decreasing and continuous on  $[0, +\infty)$ , and since for every  $p \geq 0$ ,  $\theta E_{\min}^{p+1}(\tilde{c}_p) = 0$ ,  $\tilde{c}_p$  is the unique zero in  $[0, +\infty)$  of the function  $\theta V_0 \mapsto \theta E_{\min}^{p+1}(\theta V_0)$ .  $\square$

The estimates in Propositions 12, 13 and 14 combined with the intervals given in Lemma 2 lead to the proof of Theorem 4. Before that, we prove a technical lemma.

**Lemma 6.** *For every  $y \in \mathbb{R}_+^*$ , let  $I(y) = (\frac{9}{4})^{\frac{2}{3}} \frac{y^{\frac{3}{2}+1}}{y^2+y+1}$ . Then, for every  $\eta > 0$  and every real numbers  $0 < b < a$  such that  $\frac{a-b}{b} \in [0, \eta]$ ,*

$$(a-b)b^{-\frac{1}{3}}I((1+\eta)^{\frac{2}{3}}) \leq (\frac{3}{2}a)^{\frac{2}{3}} - (\frac{3}{2}b)^{\frac{2}{3}} \leq (a-b)b^{-\frac{1}{3}}I(1). \quad (105)$$

*Proof:* One checks that  $I(1) = (\frac{3}{2})^{\frac{1}{3}}$ ,  $I'(1) = -\frac{1}{6}$  and

$$\forall y > 0, I'(y) = -\frac{\frac{3}{2} + (z-1)(\frac{1}{2} + 2z + \frac{1}{2}(1+z)z^3)}{(1+z^2+z^4)^2}, \quad \text{where } z^2 = y.$$

Hence  $I'(y) < 0$  for  $y > 1$  and  $I$  is strictly decreasing on  $[1, 1+\eta]$  for all  $\eta > 0$ .

In particular, for every real numbers  $0 < b < a$  such that  $\frac{a-b}{b} \in [0, \eta]$ ,  $(\frac{a}{b})^{\frac{2}{3}} \in [1, (1+\eta)^{\frac{2}{3}}] \subset [1, 1+\eta]$  and

$$I((1+\eta)^{\frac{2}{3}}) \leq I\left(\left(\frac{a}{b}\right)^{\frac{2}{3}}\right) \leq I(1).$$

Since

$$I\left(\left(\frac{a}{b}\right)^{\frac{2}{3}}\right) = (a-b)^{-1} \left( (\frac{3}{2}a)^{\frac{2}{3}} - (\frac{3}{2}b)^{\frac{2}{3}} \right) b^{\frac{1}{3}},$$

we get (105).  $\square$

*Proof:* (of Theorem 4). Let  $\theta V_0 > c_0$ . Let  $k_0$  defined in (8). The first point in Theorem 4 is a direct consequence of point (1) of Proposition 14 and Propositions 12 and 13 which ensure that for every  $k \in \{0, \dots, k_0\}$ ,  $\hat{E}_k$  and  $\check{E}_k$  are in  $[-V_0, 0]$ . For the second point, using Propositions 12, 13 and 14 one deduces that

$$\forall p \in \{2, \dots, k_0\}, \tilde{c}_p - c_p \leq \theta(E_{\min}^{p+1} - E_{\max}^p) \leq \tilde{c}_p - \tilde{c}_{p-2}$$

and

$$\forall p \in \{2, \dots, k_0\}, 0 < \theta(E_{\max}^p - E_{\min}^p) \leq c_p - \tilde{c}_{p-1}.$$

Let  $p \in \{2, \dots, k_0\}$ . Assume that  $p$  is even, that is  $p = 2j$  for  $j \geq 1$ . Then,

$$\tilde{c}_{2j} - \tilde{c}_{2j-2} = \left(\frac{3}{2}\tilde{\xi}_{2j}\right)^{\frac{2}{3}} - \left(\frac{3}{2}\tilde{\xi}_{2j-2}\right)^{\frac{2}{3}}.$$

Using (53) in Lemma 2, we have  $\tilde{\xi}_{2j} - \tilde{\xi}_{2j-2} \in \left[\pi - \frac{5}{9\pi} \frac{2j}{(2j)^2-1}, \pi + \frac{5}{9\pi} \frac{2j}{(2j)^2-1}\right]$  and

$$\tilde{\xi}_{2j-2}^{-\frac{1}{3}} \leq \left(-\frac{5\pi}{12} + j\pi - \frac{5}{18\pi}\right)^{-\frac{1}{3}} \leq \left(\frac{(2j-1)\pi}{2}\right)^{-\frac{1}{3}}.$$

Thus, by Lemma 6,

$$\tilde{c}_{2j} - \tilde{c}_{2j-2} \leq \left( \pi + \frac{5}{9\pi} \frac{2j}{(2j)^2 - 1} \right) \left( \frac{3}{2} \right)^{\frac{1}{3}} \left( \frac{(2j-1)\pi}{2} \right)^{-\frac{1}{3}}.$$

If  $p$  is odd, that is  $p = 2j + 1$  for  $j \geq 1$ , then, using (55) in Lemma 2, we have  $\tilde{\xi}_{2j+1} - \tilde{\xi}_{2j-1} \in \left[ \pi - \frac{7}{3\pi} \frac{2j+1}{(2j+1)^2 - 1}, \pi + \frac{7}{3\pi} \frac{2j+1}{(2j+1)^2 - 1} \right]$  and  $\tilde{\xi}_{2j-1}^{-\frac{1}{3}} \leq \left( \frac{2j\pi}{2} \right)^{-\frac{1}{3}}$ . Thus, by Lemma 6,

$$\tilde{c}_{2j+1} - \tilde{c}_{2j-1} \leq \left( \pi + \frac{7}{3\pi} \frac{2j+1}{(2j+1)^2 - 1} \right) \left( \frac{3}{2} \right)^{\frac{1}{3}} \left( \frac{2j\pi}{2} \right)^{-\frac{1}{3}}.$$

Since  $\frac{7}{3\pi} > \frac{5}{9\pi}$ , we have

$$\forall p \in \{2, \dots, k_0\}, \tilde{c}_p - \tilde{c}_{p-2} \leq \left( \pi + \frac{7}{3\pi} \frac{p}{p^2 - 1} \right) \left( \frac{3}{\pi} \right)^{\frac{1}{3}} (p-1)^{-\frac{1}{3}}$$

which proves (13). The proof of the upper bound in (12) is similar. We estimate both  $c_{2j} - \tilde{c}_{2j-1}$  and  $c_{2j+1} - \tilde{c}_{2j}$  for  $j \geq 1$  by using (49), (55), (53) and (51) to obtain that  $\xi_{2j} - \tilde{\xi}_{2j-1} \in \left[ \frac{\pi}{3} - \frac{7}{3\pi} \frac{2j+\frac{1}{3}}{2j(2j+\frac{1}{3})}, \frac{\pi}{3} + \frac{7}{3\pi} \frac{2j+\frac{1}{3}}{2j(2j+\frac{1}{3})} \right]$  and  $\xi_{2j+1} - \tilde{\xi}_{2j} \in \left[ \frac{\pi}{3} - \frac{5}{9\pi} \frac{2j+1+\frac{1}{3}}{(2j+1)(2j+1+\frac{1}{3})}, \frac{\pi}{3} + \frac{5}{9\pi} \frac{2j+1+\frac{1}{3}}{(2j+1)(2j+1+\frac{1}{3})} \right]$ . We also have that for every  $p \in \{2, \dots, k_0\}$ ,  $\tilde{\xi}_p^{-\frac{1}{3}} \leq \left( \frac{(p+1)\pi}{2} \right)^{-\frac{1}{3}}$ . Since  $\frac{7}{3\pi} > \frac{5}{9\pi}$ , we get the upper bound of (12) by using Lemma 6.

It remains to prove the lower bound in (12). We have to find a lower bound of  $\tilde{c}_p - c_p$  for every  $p \in \{2, \dots, k_0\}$ . Using (53) and (49) we get for every  $j \geq 1$ ,

$$\tilde{\xi}_{2j} - \xi_{2j} \in \left[ \frac{\pi}{6} - \frac{229}{432\pi}, \frac{\pi}{6} + \frac{229}{432\pi} \right] \subset \left[ \frac{\pi}{9}, \frac{2\pi}{9} \right].$$

We have

$$\frac{\tilde{\xi}_{2j} - \xi_{2j}}{\xi_{2j}} \leq \frac{\frac{2\pi}{9}}{\frac{5\pi}{12} + \pi - \frac{7}{16\pi}} \leq \frac{\frac{2\pi}{9}}{\frac{17\pi}{12}} \leq \frac{8}{51} \leq \frac{1}{6}.$$

Moreover, since  $\frac{5}{6} + \frac{7}{8\pi^2} < 1$ ,

$$(\xi_{2j})^{-\frac{1}{3}} \geq \left( \frac{5\pi}{12} + \frac{2j\pi}{2} + \frac{7}{16\pi} \right)^{-\frac{1}{3}} \geq \left( \frac{\pi}{2} \right)^{-\frac{1}{3}} (2j+1)^{-\frac{1}{3}}.$$

Thus, we can take  $\eta = \frac{1}{6}$  and use the lower bound in (105) to get

$$I \left( \left( \frac{7}{6} \right)^{\frac{2}{3}} \right) \frac{2^{\frac{1}{3}} \pi^{\frac{2}{3}}}{9} (2j+1)^{-\frac{1}{3}} \leq \tilde{c}_{2j} - c_{2j}.$$

For  $p = 2j + 1$ , since  $\frac{\pi}{9} < \frac{\pi}{6} - \frac{97}{264\pi}$  and  $\frac{5}{6} + \frac{5}{33\pi^2} < 1$ , and taking  $\eta = \frac{1}{2}$ , we get a larger lower bound which is

$$I \left( \left( \frac{3}{2} \right)^{\frac{2}{3}} \right) \frac{2^{\frac{1}{3}} \pi^{\frac{2}{3}}}{9} (2j+2)^{-\frac{1}{3}} \leq \tilde{c}_{2j+1} - c_{2j+1}.$$

It allows to conclude that the lower bound valid for every  $p \in \{2, \dots, k_0\}$  is the one obtained for  $p$  even. This proves the lower bound in (12).  $\square$

*Proof:* (of Corollary 1). The integer  $k_0$  defined in (8) is equal to  $\left\lceil \frac{4}{3\pi}(\theta V_0)^{\frac{3}{2}} \right\rceil$  where, for any  $x \in \mathbb{R}$ ,  $[x]$  denotes the integer part of  $x$ . Using (12), one has:

$$\forall \theta V_0 > c_0, 0 < \frac{1}{\theta V_0} \sum_{p=2}^{k_0} \theta \delta_p \leq \frac{1}{\theta V_0} \sum_{p=2}^{k_0} \left( \frac{\pi}{3} + \frac{7}{3\pi} \frac{p + \frac{1}{3}}{p(p + \frac{2}{3})} \right) \left( \frac{3}{\pi} \right)^{\frac{1}{3}} \frac{1}{p^{\frac{1}{3}}}. \quad (106)$$

Since  $x \mapsto \frac{1}{x^{\frac{1}{3}}}$  and  $x \mapsto \frac{1}{x^{\frac{1}{3}}} \frac{x + \frac{1}{3}}{x(x + \frac{2}{3})}$  are decreasing functions on  $[1, +\infty)$ , by comparison between sums and integrals,

$$\frac{3}{2} \left( (k_0 + 1)^{\frac{2}{3}} - 2^{\frac{2}{3}} \right) \leq \sum_{p=2}^{k_0} \frac{1}{p^{\frac{1}{3}}} \leq \frac{3}{2} \left( k_0^{\frac{2}{3}} - 1 \right)$$

and

$$\int_2^{k_0+1} \frac{1}{x^{\frac{1}{3}}} \frac{x + \frac{1}{3}}{x(x + \frac{2}{3})} dx \leq \sum_{p=2}^{k_0} \frac{p + \frac{1}{3}}{p(p + \frac{2}{3})} \frac{1}{p^{\frac{1}{3}}} \leq \int_1^{k_0} \frac{1}{x^{\frac{1}{3}}} \frac{x + \frac{1}{3}}{x(x + \frac{2}{3})} dx.$$

Since

$$\begin{aligned} \int \frac{1}{x^{\frac{1}{3}}} \frac{x + \frac{1}{3}}{x(x + \frac{2}{3})} dx &= -\frac{3}{2} \frac{1}{x^{\frac{1}{3}}} - \left( \frac{3}{16} \right)^{\frac{1}{3}} \ln \left( x^{\frac{1}{3}} + \left( \frac{2}{3} \right)^{\frac{1}{3}} \right) + \\ &\quad \left( \frac{3}{27} \right)^{\frac{1}{3}} \ln \left( x^{\frac{2}{3}} - \left( \frac{2}{3} x \right)^{\frac{1}{3}} + \left( \frac{2}{3} \right)^{\frac{2}{3}} \right) + \frac{3^{\frac{5}{6}}}{2^{\frac{4}{3}}} \arctan \left( \frac{2^{\frac{2}{3}}}{3^{\frac{1}{6}}} \left( x^{\frac{1}{3}} - \frac{1}{3^{\frac{1}{2}}} \right) \right), \end{aligned}$$

and  $k_0 = \left\lceil \frac{4}{3\pi}(\theta V_0)^{\frac{3}{2}} \right\rceil$ , one gets that

$$\frac{1}{\theta V_0} \sum_{p=2}^{k_0} \frac{1}{p^{\frac{1}{3}}} \xrightarrow{\theta V_0 \rightarrow +\infty} \frac{3}{2} \left( \frac{4}{3\pi} \right)^{\frac{2}{3}}$$

and

$$\frac{1}{\theta V_0} \sum_{p=2}^{k_0} \frac{p + \frac{1}{3}}{p(p + \frac{2}{3})} \frac{1}{p^{\frac{1}{3}}} \xrightarrow{\theta V_0 \rightarrow +\infty} 0.$$

Thus,

$$\frac{1}{\theta V_0} \sum_{p=2}^{k_0} \left( \frac{\pi}{3} + \frac{7}{3\pi} \frac{p + \frac{1}{3}}{p(p + \frac{2}{3})} \right) \left( \frac{3}{\pi} \right)^{\frac{1}{3}} \frac{1}{p^{\frac{1}{3}}} \xrightarrow{\theta V_0 \rightarrow +\infty} \left( \frac{2}{3} \right)^{\frac{1}{3}}. \quad (107)$$

The function  $\theta V_0 \mapsto \frac{1}{\theta V_0} \sum_{p=2}^{k_0} \theta \delta_p$  is increasing and thus admits a limit in  $\mathbb{R} \cup \{\infty\}$  at  $+\infty$ . It implies that  $D_{\theta V_0}$  also has a limit in  $\mathbb{R} \cup \{\infty\}$  at  $+\infty$  and since the upper bound in (106) has a limit in  $\mathbb{R}$  at  $+\infty$ , it is a bounded function of  $\theta V_0$  and thus  $D_{\theta V_0}$  also has a limit in  $\mathbb{R}$  when  $\theta V_0$  tends to  $+\infty$ . Then, (106) and (107) imply (14). □

## 8. SPECTRAL BANDS AND SPECTRAL GAPS IN THE SEMICLASSICAL LIMIT

Proposition 14 allows us to identify the spectral band edges among the solutions of (69), (68), (66) and (67). Using proofs similar to those of the asymptotics of  $E_{\min}^0$ ,  $E_{\max}^0$  and  $E_{\min}^1$ , one can get the following asymptotics for the spectral band edges in the semiclassical limit.

**Proposition 15.** *When  $\theta V_0$  tends to  $+\infty$ ,*

(1) *for every integer  $j \geq 0$ ,*

$$\begin{aligned} \theta E_{\min}^{2j} &= -\theta V_0 + \tilde{a}_{j+1} - \alpha\sqrt{3} \frac{(u'(-\tilde{a}_{j+1}))^2}{\tilde{a}_{j+1}} e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_{j+1})^{\frac{3}{2}}} + \\ &\mathcal{O}\left((\theta V_0 - \tilde{a}_{j+1})^{-\frac{3}{2}} e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_{j+1})^{\frac{3}{2}}}\right) \end{aligned} \quad (108)$$

and

$$\begin{aligned} \theta E_{\max}^{2j} &= -\theta V_0 + \tilde{a}_{j+1} + \alpha\sqrt{3} \frac{(u'(-\tilde{a}_{j+1}))^2}{\tilde{a}_{j+1}} e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_{j+1})^{\frac{3}{2}}} + \\ &\mathcal{O}\left((\theta V_0 - \tilde{a}_{j+1})^{-\frac{3}{2}} e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_{j+1})^{\frac{3}{2}}}\right) \end{aligned} \quad (109)$$

(2) *and for every integer  $j \geq 0$ ,*

$$\begin{aligned} \theta E_{\min}^{2j+1} &= -\theta V_0 + a_{j+1} - \alpha\sqrt{3}(u(-a_{j+1}))^2 e^{-\frac{4}{3}(\theta V_0 - a_{j+1})^{\frac{3}{2}}} + \\ &\mathcal{O}\left((\theta V_0 - a_{j+1})^{-\frac{3}{2}} e^{-\frac{4}{3}(\theta V_0 - a_{j+1})^{\frac{3}{2}}}\right) \end{aligned} \quad (110)$$

and

$$\begin{aligned} \theta E_{\max}^{2j+1} &= -\theta V_0 + a_{j+1} + \alpha\sqrt{3}(u(-a_{j+1}))^2 e^{-\frac{4}{3}(\theta V_0 - a_{j+1})^{\frac{3}{2}}} + \\ &\mathcal{O}\left((\theta V_0 - a_{j+1})^{-\frac{3}{2}} e^{-\frac{4}{3}(\theta V_0 - a_{j+1})^{\frac{3}{2}}}\right). \end{aligned} \quad (111)$$

*Proof:* For  $j = 0$  we have already obtained the asymptotic of  $E_{\min}^0$ . For every  $j \geq 1$ ,  $E_{\min}^{2j}$  is the unique solution of (66) with  $-\theta V_0 - \theta E_{\min}^{2j} \in [-\tilde{a}_{j+1}, -\tilde{c}_{2j-1}]$ . Since  $\psi^{2j-1}$  is strictly decreasing on  $[0, +\infty)$ , one can assume that  $-\theta V_0 - \theta E_{\min}^{2j} \in \left[-\tilde{a}_{j+1}, \frac{-\tilde{c}_{2j-1} - \tilde{a}_{j+1}}{2}\right]$  and on this reduced interval, the function  $x \mapsto -\frac{x}{(u'(x))^2}$  is greater than a strictly positive constant. Thus, the scheme of the proof of the asymptotics of  $E_{\min}^0$  can be followed and leads to (108).

For every  $j \geq 0$ ,  $E_{\max}^{2j}$  is the unique solution of (68) with  $-\theta V_0 - \theta E_{\max}^{2j} \in [-c_{2j}, -\tilde{a}_{j+1}]$ . Since the function  $x \mapsto -\frac{x}{(u'(x))^2}$  is greater than a strictly positive constant on the interval  $[-c_{2j}, -\tilde{a}_{j+1}]$ . Thus, the scheme of the proof of the asymptotics of  $E_{\max}^0$  can be followed and leads to (109).

For every  $j \geq 0$ ,  $E_{\min}^{2j+1}$  is the unique solution of (69) with  $-\theta V_0 - \theta E_{\min}^{2j+1} \in [-a_{j+1}, -\tilde{c}_{2j}]$ . Since  $\psi^{2j}$  is strictly decreasing on  $[0, +\infty)$ , one can assume that  $-\theta V_0 - \theta E_{\min}^{2j+1} \in \left[-a_{j+1}, \frac{-\tilde{c}_{2j} - \tilde{a}_{j+1}}{2}\right]$  and on this reduced interval, the function  $\frac{1}{u^2}$  is greater than a strictly positive constant. Thus, the scheme of the proof of the asymptotic of  $E_{\min}^1$  can be followed and leads to (110).

For every  $j \geq 0$ ,  $E_{\max}^{2j+1}$  is the unique solution of (67) with  $-\theta V_0 - \theta E_{\max}^{2j+1} \in [-c_{2j+1}, -a_{j+1}]$ . Since the function  $\frac{1}{u^2}$  is greater than a strictly positive constant on the interval  $[-c_{2j+1}, -a_{j+1}]$ . Thus, combining the proofs of the asymptotics of  $E_{\max}^0$  and  $E_{\min}^1$  leads to (109).  $\square$

These asymptotics lead to the asymptotics of the widths of the  $p$ -th spectral band and the  $p$ -th gap in the semiclassical limit.

**Proposition 16.** *When  $\theta V_0$  tends to  $+\infty$ , for every  $j \geq 0$ ,*

$$\begin{aligned} \theta\delta_{2j} &= \theta E_{\max}^{2j} - \theta E_{\min}^{2j} \\ &= 2\alpha\sqrt{3}\frac{(u'(-\tilde{a}_{j+1}))^2}{\tilde{a}_{j+1}}e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_{j+1})^{\frac{3}{2}}}\left(1 + \mathcal{O}\left((\theta V_0 - \tilde{a}_{j+1})^{-\frac{3}{2}}\right)\right), \end{aligned} \quad (112)$$

$$\begin{aligned} \theta\delta_{2j+1} &= \theta E_{\max}^{2j+1} - \theta E_{\min}^{2j+1} \\ &= 2\alpha\sqrt{3}(u(-a_{j+1}))^2e^{-\frac{4}{3}(\theta V_0 - a_{j+1})^{\frac{3}{2}}}\left(1 + \mathcal{O}\left((\theta V_0 - a_{j+1})^{-\frac{3}{2}}\right)\right). \end{aligned} \quad (113)$$

*Proof:* The asymptotic formula (112) is obtained from (108), (109) and the asymptotic formula (113) is a direct consequence of (111) and (110).  $\square$

Proposition 15 and Proposition 16 together imply Theorem 6.

*Proof:* of Theorem 6. The first statement of Theorem 6 is about the convergence of the rescaled spectral bands to the zeroes of the Airy function  $Ai$  and of its derivative, and is a consequence of the first two terms of the asymptotic developments (108), (109), (110) and (111). More precisely, for every  $j \geq 0$ ,

$$\theta V_0 + \theta E_{\min}^{2j} = \tilde{a}_{j+1} + \mathcal{O}\left(e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_{j+1})^{\frac{3}{2}}}\right)$$

and

$$\theta V_0 + \theta E_{\max}^{2j} = \tilde{a}_{j+1} + \mathcal{O}\left(e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_{j+1})^{\frac{3}{2}}}\right)$$

and both  $\theta V_0 + \theta E_{\min}^{2j}$  and  $\theta V_0 + \theta E_{\max}^{2j}$  tends to  $\tilde{a}_{j+1}$  when  $\theta V_0$  tends to  $+\infty$ .

Using (110) and (111) we prove similarly that both  $\theta V_0 + \theta E_{\min}^{2j+1}$  and  $\theta V_0 + \theta E_{\max}^{2j+1}$  tends to  $a_{j+1}$  when  $\theta V_0$  tends to  $+\infty$ .

The asymptotic formula for  $\theta\delta_{2j}$  and  $\theta\delta_{2j+1}$  in Theorem 6 are exactly the same as those in Proposition 16.  $\square$

**Proposition 17.** *When  $\theta V_0$  tends to  $+\infty$ , for every  $j \geq 0$ ,*

$$\begin{aligned} \theta\gamma_{2j} &= \theta E_{\min}^{2j+1} - \theta E_{\max}^{2j} \\ &= a_{j+1} - \tilde{a}_{j+1} - \alpha\sqrt{3}(u(-a_{j+1}))^2e^{-\frac{4}{3}(\theta V_0 - a_{j+1})^{\frac{3}{2}}}\left(1 + \mathcal{O}\left((\theta V_0 - a_{j+1})^{-\frac{3}{2}}\right)\right), \end{aligned} \quad (114)$$

and

$$\begin{aligned} \theta\gamma_{2j+1} &= \theta E_{\min}^{2j+2} - \theta E_{\max}^{2j+1} \\ &= \tilde{a}_{j+2} - a_{j+1} - \alpha\sqrt{3}\frac{(u'(-\tilde{a}_{j+2}))^2}{\tilde{a}_{j+2}}e^{-\frac{4}{3}(\theta V_0 - \tilde{a}_{j+2})^{\frac{3}{2}}}\left(1 + \mathcal{O}\left((\theta V_0 - \tilde{a}_{j+2})^{-\frac{3}{2}}\right)\right). \end{aligned} \quad (115)$$

*Proof:* The asymptotic formula (114) is a consequence of (110), (109) and the fact that  $a_{j+1} > \tilde{a}_{j+1}$ .

The asymptotic formula (115) is a consequence of (108), (111) and the fact that  $\tilde{a}_{j+2} > a_{j+1}$ .  $\square$

This proposition implies directly Theorem 7 of the introduction.

## 9. CONCLUSION

Let us summarize some of the results we have obtained in this article.

- (1) We have been able to get very precise estimates of the widths of the spectral bands and the spectral gaps in the semiclassical limit for a periodic potential which is not analytic and not even differentiable at its maxima or minima. Up to our knowledge, this is the first example of non-regular periodic potential for which such estimates have been obtained. This was done thanks to the accurate asymptotic expansions of the classical Airy functions and their derivatives and thanks to a bootstrap analysis argument developed in the proof of Theorem 3.
- (2) We defined a semiclassical regime which is not the semiclassical limit. In this regime the results are stated for a fixed value of the semiclassical parameter  $\theta V_0$ . This regime is characterized by the comparison between  $\theta V_0$  and the constant  $c_0$ : if  $\theta V_0 > c_0$  then the periodic Airy-Schrödinger operator is in the semiclassical regime. Here,  $c_0$  is explicitly defined and we even know an approximate value:  $c_0 \simeq 1.515$ .
- (3) In the semiclassical regime, we count the number of spectral bands which lie in the range of the potential  $V$ . This number depends only of the value of the semiclassical parameter  $\theta V_0$  compared to the values of the zeroes of the canonical solutions of the Airy equation and their derivatives. In Theorem 5 we give a dynamical picture of the successive entrances in the range of  $V$  of the spectral bands and gaps when  $\theta V_0$  grows and takes the successive values  $c_k$  and  $\tilde{c}_k$  for any  $k \geq 0$ .
- (4) In the semiclassical regime, we estimate the widths of the spectral bands and gaps which lie in the range of the potential  $V$ . The bounds for the  $p$ -th spectral band or gap depend only on  $p$ .
- (5) In the classical regime, which is characterized by the inequality  $\theta V_0 \leq c_0$ , we give a complete description of the first spectral band. We also get the behaviour of this first spectral band in the classical limit, that is when  $\theta V_0$  tends to 0.

## APPENDIX A. STURM-PICONE'S LEMMAS

In this Appendix we prove a Sturm's formula and a version of the Sturm-Picone's formula adapted to the setting of the proof of Lemma 10.

**Lemma 7.** *Let  $a < b$  be two real numbers and let  $g_1, g_2 \in C^0([a, b])$ . Let  $z$  be a solution of  $-z'' + g_1 z = 0$  and let  $y$  be a solution of  $-y'' + g_2 y = 0$ . Then:*

$$(yz' - zy')' = (g_1 - g_2)yz. \quad (116)$$

*Proof:* We have:

$$y(-z'' + g_1 z) - z(-y'' + g_2 y) = -yz'' + zy'' = -(yz' - zy')'$$

We also have:

$$(-y'' + g_1 y) - (-y'' + g_2 y) = (g_1 - g_2)y.$$

Then,

$$y(-z'' + g_1 z) - z(-z'' + g_2 z + (g_1 - g_2)y) = -(yz' - zy')'.$$

Since  $-z'' + g_1 z = 0$  and  $-y'' + g_2 y = 0$ , we finally have:

$$-(yz' - zy')' = -(g_1 - g_2)yz,$$

which proves (116).  $\square$

**Lemma 8.** *Let  $a < b$  be two real numbers and let  $q_1, q_2, g \in C^0([a, b]) \cap C^1((a, b))$ ,  $q_1 > q_2 > 0$ . Let  $z$  be a solution of  $-(q_1 z')' + g z = 0$  and let  $y$  be a solution of  $-(q_2 y')' + g y = 0$  with  $y > 0$  on  $(a, b]$ . Then:*

$$\left( \frac{z}{y} (q_1 y z' - q_2 y' z) \right)' = (q_1 - q_2) (z')^2 + q_2 \left( z' - \frac{y' z}{y} \right)^2. \quad (117)$$

Moreover, if there exists  $\eta > 0$  such that  $q_1 - q_2 > \eta$ , then there exists  $A > 0$  such that

$$\left[ \frac{z}{y} (q_1 y z' - q_2 y' z) \right]_a^b \geq A \int_a^b z^2(x) dx. \quad (118)$$

*Proof:* We have, on the interval  $(a, b)$ ,

$$\begin{aligned} \left( \frac{z}{y} (q_1 y z' - q_2 y' z) \right)' &= \left( q_1 z z' - q_2 \frac{y'}{y} z^2 \right)' \\ &= (q_1 z')' z + q_1 (z')^2 - (q_2 y')' \frac{z^2}{y} - q_2 y' \left( \frac{z^2}{y} \right)' \\ &= g z^2 + q_1 (z')^2 - g y \frac{z^2}{y} - q_2 y' \left( \frac{z^2}{y} \right)' \\ &= q_1 (z')^2 - q_2 y' \left( \frac{z^2}{y} \right)' \\ &= (q_1 - q_2) (z')^2 + q_2 \left( (z')^2 - y' \left( \frac{z^2}{y} \right)' \right) \\ &= (q_1 - q_2) (z')^2 + q_2 \left( (z')^2 - 2y' \frac{z z'}{y} + \frac{(y')^2}{y^2} z^2 \right) \\ &= (q_1 - q_2) (z')^2 + q_2 \left( z' - \frac{y' z}{y} \right)^2. \end{aligned}$$

This proves (117). Then, integrating (117) between  $a$  and  $b$  and using Poincaré inequality in the last inequality, there exists  $A > 0$  (depending on  $\eta, a$  and  $b$ ) such that

$$\begin{aligned} \left[ \frac{z}{y} (q_1 y z' - q_2 y' z) \right]_a^b &= \int_a^b (q_1(x) - q_2(x)) (z'(x))^2 + q_2(x) \left( z'(x) - \frac{y'(x) z(x)}{y(x)} \right)^2 dx \\ &\geq \int_a^b (q_1(x) - q_2(x)) (z'(x))^2 dx \\ &\geq \eta \int_a^b (z'(x))^2 dx \geq A \int_a^b (z(x))^2 dx. \end{aligned}$$

This proves (118).  $\square$



## APPENDIX B. THE MONOTONICITY ARGUMENTS

We have defined the functions  $f_x$ ,  $g_x$  and the functions  $z_k$  for  $k \geq 0$  in Section 5.3.

**Lemma 9.** *Let  $k \geq 0$ . Then, for every  $x \geq 0$ ,*

$$z_k(x) \geq 0 \quad \text{and} \quad z_k(x) = x - \psi_k(x).$$

Therefore,  $z_k$  is continuous on  $[0, +\infty)$ . Moreover, for every  $j \geq 0$  and every  $x \geq 0$ ,

$$\begin{aligned} 0 < x + \tilde{a}_1 < z_0(x) \leq x + c_0 < \dots < x + \tilde{a}_{j+1} < z_{2j}(x) \leq x + c_{2j} \\ < x + a_{j+1} < z_{2j+1}(x) \leq x + c_{2j+1} \dots \end{aligned} \quad (119)$$

*Proof:* In this proof it will be easier to use the expressions in terms of classical Airy functions for  $f_x$  and  $g_x$  since we will use classical properties of the  $Ai$  and  $Bi$  functions and in particular the fact that  $Ai'$  is strictly negative on the positive real half-line, which is not the case for  $u'$ .

For  $x \geq 0$ ,  $Ai(x) > 0$ ,  $Bi(x) > 0$ ,  $Bi'$  is strictly positive on  $[0, +\infty)$  and  $Ai'$  is strictly negative on  $[0, +\infty)$ . If  $z \leq 0$ ,  $x - z \geq 0$  and  $f_x(z) > 0$ . Thus,  $z_0(x) > 0$ . Then, 0 is a zero of  $g_x$  and since  $\frac{Bi}{Ai}$  is strictly increasing on  $[0, +\infty)$ , and for  $z < 0$ ,  $x - z > x$  and  $g_x(z) > 0$ . So, 0 is the first zero of  $g_x$ . In particular, for every  $k \geq 0$ ,  $z_k(x) \geq 0$ .

Let  $j \geq 0$ . We remark that, by definition of  $\psi_{2j}$ , we have  $f_x(x - \psi_{2j}(x)) = 0$ , and by definition of  $\psi_{2j+1}$ , we have  $g_x(x - \psi_{2j+1}(x)) = 0$ . Moreover, for  $x - z \notin \{-\tilde{c}_{2j+1}\}_{j \geq 0}$ , by unicity of  $\psi_{2j}(x)$  in  $[-c_{2j}, -\tilde{a}_{j+1})$ ,  $x - \psi_{2j}(x)$  is the unique zero of  $f_x$  in  $(x + \tilde{a}_{j+1}, x + c_{2j}]$ . Since we have  $f_x(x + \tilde{a}_{j+1}) = Bi'(-\tilde{a}_{j+1})Ai(x) \neq 0$ , the set of the zeroes of  $f_x$  is exactly  $\{x - \psi_{2j}(x), j \geq 0\}$ . Thus, for every  $j \geq 0$ ,  $z_{2j}(x) = x - \psi_{2j}(x)$ .

For  $x - z \notin \{-\tilde{c}_{2j}\}_{j \geq 0}$ , by unicity of  $\psi_{2j+1}(x)$  in  $[-c_{2j+1}, -a_{j+1})$ ,  $x - \psi_{2j+1}(x)$  is the unique zero of  $g_x$  in  $(x + a_{j+1}, x + c_{2j+1}]$ . Since we have  $g_x(x + a_{j+1}) = Bi(-a_{j+1})Ai(x) \neq 0$ , the set of the zeroes of  $g_x$  is exactly  $\{0\} \cup \{x - \psi_{2j+1}(x), j \geq 0\}$ . Thus, for every  $j \geq 0$ ,  $z_{2j+1}(x) = x - \psi_{2j+1}(x)$ .

By Lemma 3, we deduce that  $z_k$  is continuous on  $[0, +\infty)$ . Since for every  $j \geq 0$ ,  $\psi_{2j}(x) \in [-c_{2j}, -\tilde{a}_{j+1})$  and  $\psi_{2j+1}(x) \in [-c_{2j+1}, -a_{j+1})$ , we deduce (119).  $\square$

We can now prove further properties of the functions  $f_x$  and  $g_x$  and in particular their signs and their variations.

**Proposition 18.** *For every  $x \geq 0$ , the functions  $f_x$  and  $g_x$  from  $\mathbb{R}$  to  $\mathbb{R}$  have the following properties:*

- (1)  $\forall z \in \mathbb{R}$ ,  $g'_x(z) = -f_x(z)$  and  $f'_x(z) = -(x - z)g_x(z)$ .
- (2)  $f_x$  satisfies the ordinary differential equation on  $\mathbb{R} \setminus \{x\}$ :

$$\left( \frac{f'_x}{x - z} \right)' = f_x, \quad (120)$$

and  $g_x$  satisfies the Airy equation:  $g''_x = (x - z)g_x$ .

*Proof:* We compute the derivative of  $f_x$ , using the fact that  $u$  and  $v$  satisfies the Airy equation:

$$\forall z \in \mathbb{R}, f'_x(z) = (x - z)(u(x - z)v(x) - v(x - z)u(x)). \quad (121)$$

Thus,  $f'_x(z) = -(x-z)g_x(z)$ , for every  $z \in \mathbb{R}$ . A direct computation leads to  $g'_x(z) = -f_x(z)$ , for every  $z \in \mathbb{R}$ .

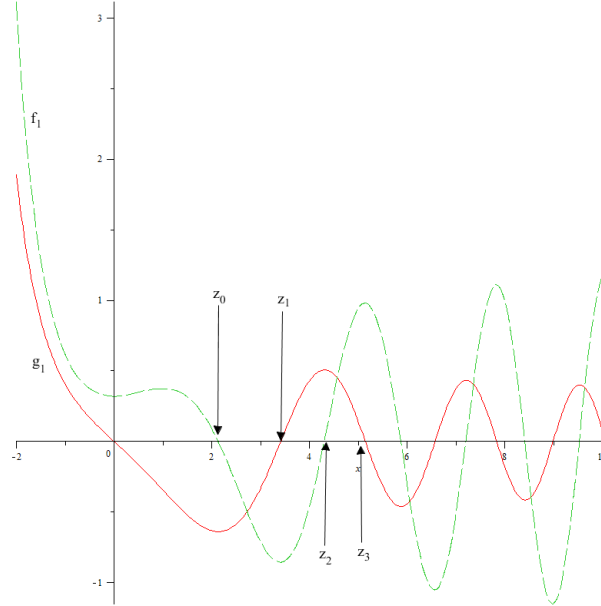
For the second point, we assume that  $z \neq x$ , we divide (121) by  $x-z$  and by derivation:

$$\forall z \in \mathbb{R} \setminus \{x\}, \left( \frac{f'_x}{x-z} \right)' = -u'(x-z)v(x) + v'(x-z)u(x) = f_x(z).$$

The function  $g_x$  satisfies the Airy equation since it is a linear combination of solutions of the Airy equation. □

**Proposition 19.** *For every  $x \geq 0$ , the functions  $f_x$  and  $g_x$  from  $\mathbb{R}$  to  $\mathbb{R}$  have the following properties:*

- (1) *The function  $f'_x$  vanishes exactly on  $0, x$ , and  $z_{2j+1}(x)$  for every  $j \geq 0$ . It is strictly negative on  $(-\infty, 0)$ , strictly positive on  $(0, x)$ , strictly negative on  $(x, z_1(x))$  and, for every  $j \geq 1$ ,  $(-1)^{j+1}f'_x$  is strictly positive on  $(z_{2j-1}(x), z_{2j+1}(x))$ .*
- (2) *The function  $f_x$  is strictly positive on  $(-\infty, z_0(x))$  and, for every  $j \geq 1$ ,  $(-1)^{j+1}f_x$  is strictly positive on  $(z_{2j-2}(x), z_{2j}(x))$ .*
- (3) *The function  $g'_x$  vanishes exactly on  $z_{2j}(x)$  for every  $j \geq 0$ . It is strictly negative on  $(-\infty, z_0(x))$  and, for every  $j \geq 1$ ,  $(-1)^{j+1}g'_x$  is strictly positive on  $(z_{2j-2}(x), z_{2j}(x))$ .*
- (4) *The function  $g_x$  is strictly positive on  $(-\infty, 0)$ , strictly negative on  $(0, z_1(x))$  and, for every  $j \geq 1$ ,  $(-1)^{j+1}g_x$  is strictly positive on  $(z_{2j-1}, z_{2j+1})$ .*



*Proof:* We will again use the expressions in terms of classical Airy functions for  $f_x$  and  $g_x$ .

(1) From (121), it is clear that  $f'_x(0) = f'_x(x) = 0$ . We have already proven in Lemma 4 that for  $z \in (-\infty, 0)$ ,  $f'_x(z) < 0$ . Then, for  $z \in (0, x)$ ,  $x - z > 0$ ,  $x - z < x$ ,  $\frac{Bi}{Ai}(x - z) < \frac{Bi}{Ai}(x)$  and  $f'_x(z) > 0$ . From  $f'_x(z) = -(x - z)g_x(z)$  and Lemma 4, we know that the remaining zeroes of  $f'_x$  are exactly the  $z_{2j+1}(x)$  for  $j \geq 0$ . We also have  $f'_x(x + a_1) = a_1 Bi(-a_1) Ai(x)$  with  $a_1 > 0$ ,  $Bi(-a_1) < 0$  and  $Ai(x) > 0$ , thus  $f'_x(x + a_1) < 0$ . Since  $f'_x$  is of constant sign in  $(x, z_1(x))$ , one deduce that  $f'_x$  is strictly negative on  $(x, z_1(x))$ . To finish the proof of point 1, it is sufficient to remark that  $f'_x$  is of constant sign on every interval  $(z_{2j-1}(x), z_{2j+1}(x))$  for  $j \geq 1$ . But,  $x + a_{2j} \in (z_{4j-3}(x), z_{4j-1}(x))$  and  $f'_x(x + a_{2j}) = a_{2j} Bi(-a_{2j}) Ai(x) > 0$ , since  $Bi(-a_{2j}) > 0$ . Thus,  $f'_x$  is strictly positive on  $(z_{4j-3}(x), z_{4j-1}(x))$ . Similarly,  $x + a_{2j+1} \in (z_{4j-1}(x), z_{4j+1}(x))$  and  $f'_x(x + a_{2j+1}) = a_{2j+1} Bi(-a_{2j+1}) Ai(x) < 0$ , since  $Bi(-a_{2j+1}) < 0$ . Thus,  $f'_x$  is strictly negative on  $(z_{4j-1}(x), z_{4j+1}(x))$ .

(2) We have already proven in Lemma 4 that for  $z \in (-\infty, 0)$ ,  $f_x(z) > 0$ . We also have  $f_x(0) = \frac{1}{\pi} > 0$  since it is the value of the Wronskian of  $Ai$  and  $Bi$  and thus, for every  $z \in (-\infty, x)$ ,  $f_x(z) \geq \frac{1}{\pi}$ . Since  $z_0(x)$  is the first zero of  $f_x$ , this function is strictly positive on  $(-\infty, z_0(x))$ . We remark that  $f_x$  is of constant sign on every interval  $(z_{2j-2}(x), z_{2j}(x))$  for  $j \geq 1$ . But,  $x + \tilde{a}_{2j+1} \in (z_{4j-2}(x), z_{4j}(x))$  and  $f_x(x + \tilde{a}_{2j+1}) = Bi'(-\tilde{a}_{2j+1}) Ai(x) > 0$ , since  $Bi'(-\tilde{a}_{2j+1}) > 0$ . Thus,  $f_x$  is strictly positive on  $(z_{4j-2}(x), z_{4j}(x))$ . Similarly,  $x + \tilde{a}_{2j+2} \in (z_{4j}(x), z_{4j+2}(x))$  and  $f_x(x + \tilde{a}_{2j+2}) = Bi'(-\tilde{a}_{2j+2}) Ai(x) < 0$ , since  $Bi'(-\tilde{a}_{2j+2}) < 0$ . Thus,  $f_x$  is strictly negative on  $(z_{4j}(x), z_{4j+2}(x))$ .

(3) It is deduced directly from point 1 of Proposition 18 and point 2.

(4) It comes from point 1 of Proposition 18, point 1 and the fact that for  $z \geq z_1(x)$ ,  $z > x$  and  $x - z < 0$ . □

We have now all the ingredients needed to prove that  $z_k$  is a strictly increasing function.

**Lemma 10.** *For every  $k \geq 0$ , the function  $z_k$  is strictly increasing from  $[0, +\infty)$  to  $[c_k, +\infty)$ .*

*Proof:* We will separate the proof in two cases, depending on the parity of  $k$ .

**Case 1:**  $k = 2j$  for  $j \geq 0$ . Let  $0 < x_1 < x_2$ . We want to prove that  $z_{2j}(x_1) \leq z_{2j}(x_2)$ . Assume that  $z_{2j}(x_2) < z_{2j}(x_1)$ . Let  $\delta > 0$  be such that  $z_{2j}(x_2) + \delta < z_{2j}(x_1)$ . We use (119) to get

$$z_{2j-1}(x_1) < x_1 + \tilde{a}_{j+1} < x_2 + \tilde{a}_{j+1} < z_{2j}(x_2) < z_{2j}(x_2) + \delta <$$

$$z_{2j}(x_1) < x_1 + a_{j+1} < x_2 + a_{j+1} < z_{2j+1}(x_2).$$

In particular,  $x_1 - (z_{2j}(x_2) + \delta) < 0$ ,  $x_2 - (z_{2j}(x_2) + \delta) < 0$  and

$$(z_{2j}(x_2) + \delta) \in (z_{2j-1}(x_1), z_{2j}(x_1)) \cap (z_{2j}(x_2), z_{2j+1}(x_2)).$$

Thus, using Proposition 19,

$$(-1)^j f_{x_1}(z_{2j}(x_2) + \delta) > 0, \quad (-1)^j f'_{x_1}(z_{2j}(x_2) + \delta) < 0, \quad (122)$$

$$\text{and} \quad (-1)^j f_{x_2}(z_{2j}(x_2) + \delta) < 0, \quad (-1)^j f'_{x_2}(z_{2j}(x_2) + \delta) < 0. \quad (123)$$

There exists  $\eta > 0$  such that, for every  $z \in [z_{2j}(x_2) + \delta, z_{2j}(x_1)]$ ,  $\frac{1}{x_1-z} - \frac{1}{x_2-z} \geq \eta$ . Moreover, since  $(z_{2j}(x_2) + \delta, z_{2j}(x_1)) \subset (z_{2j-1}(x_1), z_{2j}(x_1))$ , for every  $z \in (z_{2j}(x_2) + \delta, z_{2j}(x_1))$ ,  $(-1)^{j+1}f_{x_1}(z) > 0$ . Similarly, since  $(z_{2j}(x_2) + \delta, z_{2j}(x_1)) \subset (z_{2j}(x_2), z_{2j+1}(x_2))$ , for every  $z \in (z_{2j}(x_2) + \delta, z_{2j}(x_1))$ ,  $(-1)^{j+1}f_{x_2}(z) < 0$ . Then, applying Lemma 8,

$$\int_{z_{2j}(x_2)+\delta}^{z_{2j}(x_1)} \left( \frac{f_{x_1}(z)}{f_{x_2}(z)} \left( \frac{f'_{x_1}(z)f_{x_2}(z)}{x_1-z} - \frac{f_{x_1}(z)f'_{x_2}(z)}{x_2-z} \right) \right)' dz > 0. \quad (124)$$

Since  $f_{x_1}(z_{2j}(x_1)) = 0$ , the integral in the left side of equality (124) is equal to

$$-\frac{f_{x_1}(z_{2j}(x_2) + \delta)f'_{x_1}(z_{2j}(x_2) + \delta)}{x_1 - z_{2j}(x_2) - \delta} + \frac{f_{x_1}^2(z_{2j}(x_2) + \delta)}{x_2 - z_{2j}(x_2) - \delta} \cdot \frac{f'_{x_2}(z_{2j}(x_2) + \delta)}{f_{x_2}(z_{2j}(x_2) + \delta)} < 0 \quad (125)$$

by the use of (122) and (123). But (125) contradicts (124) and thus we must have  $z_{2j}(x_1) \leq z_{2j}(x_2)$ . The function  $z_{2j}$  is an increasing function from  $[0, +\infty)$  to  $[c_k, +\infty)$ .

It remains to prove that  $z_{2j}$  is strictly increasing. If  $z_{2j}$  is not strictly increasing, since it is increasing and continuous, there exists an interval in  $[0, +\infty)$  on which  $z_{2j}$  is constant. But,  $z_{2j}$  is also analytic on  $[0, +\infty)$  since one can prove that actually the functions  $\psi_{2j}$  are analytic. Thus, if it is constant on an interval, it should be constant everywhere which is not the case, so  $z_{2j}$  is actually strictly increasing.

**Case 2:**  $k = 2j + 1$  for  $j \geq 0$ . Let  $x_1 < x_2$ . We will show by induction on  $j \geq 0$  that  $z_{2j+1}(x_1) < z_{2j+1}(x_2)$ .

For  $j = 0$ , we can directly apply the classical interlacing zeroes theorem of Sturm with potentials  $q(z) = -(x_2 - z) < p(z) = -(x_1 - z)$ , since  $g_{x_1}$  satisfies  $-g''_{x_1} + pg_{x_1} = 0$  and  $g_{x_2}$  satisfies  $-g''_{x_2} + qg_{x_2} = 0$ . Applying this theorem between 0 which is a common zero to  $g_{x_1}$  and  $g_{x_2}$  and  $z_1(x_2)$  which is the first strictly positive zero of  $g_{x_2}$  one gets that  $g_{x_1}$  admits a zero in the interval  $(0, z_1(x_2))$ . Since  $z_1(x_1)$  is the smallest strictly positive zero of  $g_{x_1}$ , we necessarily have  $z_1(x_1) \in (0, z_1(x_2))$  and  $z_1(x_1) < z_1(x_2)$ . Thus,  $z_1$  is strictly increasing.

Let  $j \geq 1$ . We assume by induction that  $z_{2j-1}(x_1) < z_{2j-1}(x_2)$  and we want to prove that  $z_{2j+1}(x_1) < z_{2j+1}(x_2)$ . We assume the contrary:  $z_{2j+1}(x_2) \leq z_{2j+1}(x_1)$ . Then we have

$$z_{2j-1}(x_1) < z_{2j-1}(x_2) < z_{2j}(x_2) < z_{2j+1}(x_2) \leq z_{2j+1}(x_1). \quad (126)$$

We apply Lemma 7 to  $g_{x_1}$  and  $g_{x_2}$  between  $z_{2j-1}(x_2)$  and  $z_{2j+1}(x_2)$  to get

$$\int_{z_{2j-1}(x_2)}^{z_{2j+1}(x_2)} (g_{x_2}(z)g'_{x_1}(z) - g_{x_1}(z)g'_{x_2}(z))' dz = \int_{z_{2j-1}(x_2)}^{z_{2j+1}(x_2)} (x_1 - x_2)g_{x_1}(z)g_{x_2}(z) dz. \quad (127)$$

But, using (126), we have  $(z_{2j-1}(x_2), z_{2j+1}(x_2)) \subset (z_{2j-1}(x_1), z_{2j+1}(x_1))$ . Using Proposition 19,

$$\forall z \in (z_{2j-1}(x_2), z_{2j+1}(x_2)), \quad (-1)^j g_{x_1}(z) < 0 \quad \text{and} \quad (-1)^j g_{x_2}(z) < 0.$$

Since  $x_1 - x_2 < 0$ ,

$$\int_{z_{2j-1}(x_2)}^{z_{2j+1}(x_2)} (x_1 - x_2)g_{x_1}(z)g_{x_2}(z) dz < 0. \quad (128)$$

We have,

$$\int_{z_{2j-1}(x_2)}^{z_{2j+1}(x_2)} (g_{x_2}(z)g'_{x_1}(z) - g_{x_1}g'_{x_2}(z))' dz = \\ - g_{x_1}(z_{2j+1}(x_2))g'_{x_2}(z_{2j+1}(x_2)) + g_{x_1}(z_{2j-1}(x_2))g'_{x_2}(z_{2j-1}(x_2)).$$

But, using again Proposition 19,

$$\forall z \in [z_{2j-1}(x_2), z_{2j}(x_2)], \quad (-1)^j g'_{x_2}(z) < 0$$

and

$$\forall z \in (z_{2j}(x_2), z_{2j+1}(x_2)], \quad (-1)^j g'_{x_2}(z) > 0.$$

In particular,

$$(-1)^j g_{x_1}(z_{2j+1}(x_2)) < 0, \quad (-1)^j g'_{x_2}(z_{2j+1}(x_2)) > 0,$$

and

$$(-1)^j g_{x_1}(z_{2j-1}(x_2)) < 0, \quad (-1)^j g'_{x_2}(z_{2j-1}(x_2)) < 0.$$

Thus,

$$\int_{z_{2j-1}(x_2)}^{z_{2j+1}(x_2)} (g_{x_2}(z)g'_{x_1}(z) - g_{x_1}g'_{x_2}(z))' dz > 0$$

which contradicts (128). So we have  $z_{2j+1}(x_1) < z_{2j+1}(x_2)$  and  $z_{2j+1}$  is strictly increasing.

We have thus proven by induction that for every  $j \geq 0$ ,  $z_{2j+1}$  is strictly increasing from  $[0, +\infty)$  to  $[c_{2j+1}, +\infty)$ . This finishes the proof of Lemma 10.  $\square$

### APPENDIX C. EIGENVALUES AND EIGENFUNCTIONS FOR A LINEAR POTENTIAL WELL

We solve the eigenvalue problem for a linear potential well:

$$-\frac{d^2\psi}{dx^2} + |x|\psi = \lambda\psi, \quad \text{with } \lambda \in \mathbb{R}, \quad \psi \in H^2(\mathbb{R})$$

and  $\psi$  not identically zero. In particular one has  $\psi(0^+) = \psi(0^-)$  and  $\psi'(0^+) = \psi'(0^-)$  since  $\psi$  must be  $C^1$ . We solve both equations  $-\psi'' + x\psi = \lambda\psi$  for  $x > 0$  and  $-\psi'' - x\psi = \lambda\psi$  for  $x < 0$ . We get that there exists  $C, D \in \mathbb{R}$  such that

$$\forall x > 0, \quad \psi(x) = C \cdot Ai(-\lambda + x) \quad \text{and} \quad \forall x < 0, \quad \psi(x) = D \cdot Ai(-\lambda - x).$$

For  $x = 0$ ,  $C \cdot Ai(-\lambda) = D \cdot Ai(-\lambda)$  and  $C \cdot Ai'(-\lambda) = -D \cdot Ai'(-\lambda)$ . If  $Ai(-\lambda) \neq 0$  and  $Ai'(-\lambda) \neq 0$  then  $C = D = 0$  and  $\psi = 0$ .

Thus,  $Ai(-\lambda) = 0$  or  $Ai'(-\lambda) = 0$  and the eigenvalues are the opposite of the zeroes of the Airy function and its derivative, the  $a_{j+1}$  and  $\tilde{a}_{j+1}$ , for  $j \geq 0$ . These eigenvalues are of multiplicity 1.

The eigenspace associated with  $\tilde{a}_{j+1}$  is spanned by  $x \mapsto Ai(|x| - \tilde{a}_{j+1})$  and the eigenspace associated with  $a_{j+1}$  is spanned by  $x \mapsto \text{sign}(x) \cdot Ai(|x| - a_{j+1})$ .

Remark that these eigenfunctions are both decaying to 0 faster than exponentially when  $|x|$  tends to  $+\infty$ . This implies the absence of tunneling effect in the semiclassical limit.

With the first statement of Theorem 6, one deduces immediately Corollary 2.

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