

Alma Mater Studiorum Università di Bologna
Archivio istituzionale della ricerca

Molecular predissociation resonances near an energy-level crossing I: Elliptic interaction

This is the final peer-reviewed author's accepted manuscript (postprint) of the following publication:

Published Version:

Fujiie, S., Martinez, A.G., Watanabe, T. (2016). Molecular predissociation resonances near an energy-level crossing I: Elliptic interaction. JOURNAL OF DIFFERENTIAL EQUATIONS, 260(5), 4051-4085 [10.1016/j.jde.2015.11.015].

Availability:

This version is available at: <https://hdl.handle.net/11585/592075> since: 2021-07-15

Published:

DOI: <http://doi.org/10.1016/j.jde.2015.11.015>

Terms of use:

Some rights reserved. The terms and conditions for the reuse of this version of the manuscript are specified in the publishing policy. For all terms of use and more information see the publisher's website.

This item was downloaded from IRIS Università di Bologna (<https://cris.unibo.it/>).
When citing, please refer to the published version.

(Article begins on next page)

This is the final peer-reviewed accepted manuscript of:

Fujié, S., Martinez, A., & Watanabe, T. (2016). Molecular predissociation resonances near an energy-level crossing I: Elliptic interaction. Journal of Differential Equations, 260(5), 4051-4085.

The final published version is available online at: <http://dx.doi.org/10.1016/j.jde.2015.11.015>

Rights / License:

The terms and conditions for the reuse of this version of the manuscript are specified in the publishing policy. For all terms of use and more information see the publisher's website.

This item was downloaded from IRIS Università di Bologna (<https://cris.unibo.it/>)

When citing, please refer to the published version.

MOLECULAR PREDISSOCIATION RESONANCES NEAR AN ENERGY-LEVEL CROSSING I: ELLIPTIC INTERACTION

S. FUJIE¹, A. MARTINEZ² AND T. WATANABE³

ABSTRACT. We study the resonances of a two-by-two semiclassical system of one dimensional Schrödinger operators, near an energy where the two potentials intersect transversally, one of them being bonding, and the other one anti-bonding. We locate the resonances and obtain estimates on their widths, that become optimal under an additional condition of ellipticity on the interaction. Our method relies on the construction of fundamental solutions for the two scalar unperturbed operators, and on an iterative procedure in order to obtain solutions to the system.

Keywords: Resonances; Born-Oppenheimer approximation; eigenvalue crossing; Differential system.

Subject classifications: 35P15; 35C20; 35S99; 47A75.

¹Department of Mathematical Sciences, Ritsumeikan University, 1-1-1 Noji-Higashi, Kusatsu, 525-8577, Japan, fujie@fc.ritsumei.ac.jp

²Università di Bologna, Dipartimento di Matematica, Piazza di Porta San Donato, 40127 Bologna, Italy, andre.martinez@unibo.it

³Department of Mathematical Sciences, Ritsumeikan University, 1-1-1 Noji-Higashi, Kusatsu, 525-8577, Japan, t-watana@se.ritsumei.ac.jp

1. INTRODUCTION

This paper is a first attempt to study the diatomic molecular predissociation resonances in the Born-Oppenheimer approximation, at energies close to that of the crossing of the electronic levels. Our aim is to provide precise estimates both on the real parts and on the imaginary parts (widths) of the resonances. As it is well known, they respectively correspond to the radiation frequency and to the inverse of the life-time of the molecule.

The Born-Oppenheimer approximation permits to reduce the study to that of a semiclassical system of Schrödinger-type operators (see, e.g., [15, 19, 20]), the size of which depends on the number of electronic levels that are involved, and with semiclassical parameter h given by the square-root of the inverse of the (mean-) mass of the nuclei. At sufficiently low energies, this system is scalar, and, typically, one can apply the numerous results coming from the semiclassical analysis of the Schrödinger operator (see, e.e., [10, 12, 16, 22, 13, 3, 4, 25] and references therein).

On the contrary, when several electronic levels are involved, only few results are available. One may quote [2, 21, 6, 8], where very particular potentials are considered, and [18, 14, 9, 17], where the potentials are much more general, but the energy considered is lower than that of the crossing. Actually, in this last situation the widths of the resonances can be estimated by a tunnelling effect through a potential barrier, and thus are exponentially small (in the parameter h). In particular, these resonances correspond to extremely long life-times, and, from a chemical point of view, their instability is almost impossible to observe experimentally. It is therefore of interest to consider situations where the widths are not that small.

As a matter of fact, this is what is expected when the energy considered becomes very close to that of the crossing, because at such a level the potential barrier disappears. However, this case is difficult to treat in general, because it corresponds to a somehow degenerate situation where the characteristic set of the operator has a singularity of the type $\{|\xi|^4 - x_1^2 = 0\}$.

Here, we study a model with one degree of freedom, where such a phenomenon occurs. Namely, we consider a 2×2 matrix system, the diagonal part of which consists of semiclassical Schrödinger operators, and the off-diagonal part of a lower order differential interaction. We assume that the two potentials cross transversally at the origin, with value 0, and that, at this energy level, one of the two potentials admits a well, while the other one is non-trapping (see figure 1).

For such a model, we study the resonances $E = E(h)$ that have a real part $\mathcal{O}(h^{2/3})$ and an imaginary part $\mathcal{O}(h)$. We actually prove their existence, and give their asymptotic behaviours up to $\mathcal{O}(h^2)$ as $h \rightarrow 0_+$. In particular, under an additional condition of ellipticity on the interaction, we find that their widths behave exactly like $h^{5/3}$, except possibly for particular values of the limit of $h^{-2/3}E(h)$, corresponding to positive zeros of some Airy-type function, and for which the width becomes $o(h^{5/3})$. In our model, the interaction is of the form hW , with $W = r_0(x) + r_1(x)hD_x$, and the ellipticity

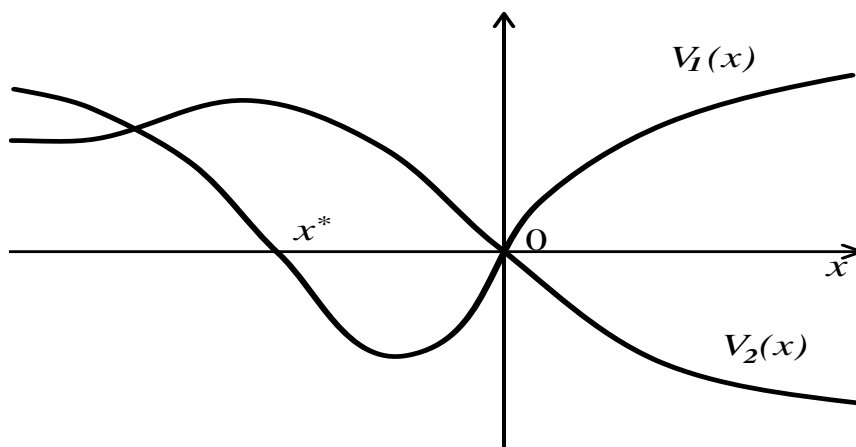


FIGURE 1. The two potentials

condition is that $r_0 \neq 0$ at the point 0 of crossing of the two energy levels. Actually, from a microlocal point of view, the interaction takes place at the point $(0, 0)$ of the phase-space, and the condition $r_0(0) \neq 0$ is nothing but the ellipticity of the symbol $r_0(x) + r_1(x)\xi$ of W at $(x, \xi) = (0, 0)$.

In a forthcoming paper, we plan to also study the case where r_0 vanishes identically, that is when the interaction is a vector-field (and thus is not anymore elliptic at $(0, 0)$). This is typically what comes out after the Feshbach reduction in the Born-Oppenheimer approximation (see, e.e., [20] and references therein).

It is important to notice that, for such a kind of system, none of the standard methods used in the scalar case can be applied. For instance, the exact WKB method (see, e.g., [7, 23]) does not work, because of the presence of 4 phase-functions $\pm\varphi_j$, $j = 1, 2$ (two for each potentials). Indeed, the method requires that, for each of them, there exists at least one direction where the real part of the difference with the three other ones increases, and here it cannot be the case. Even the formal semiclassical WKB constructions can be performed only at those points where the two potentials do not cross. Finally, the recent method proposed by D. Yafaev in [24] (and from which this work has been mostly inspired) does not seem to be adaptable to our case.

Therefore, instead of trying to generalise the scalar methods, we have chosen to use particular fundamental solutions of the two scalar underlying Schrödinger operators, and to take advantage of the fact that everything is known on their behaviours (both semiclassical and at infinity) in order to solve the system by an iterative procedure. In that way, we can construct two exponentially decaying solutions on one side, and two outgoing solutions on the other side, with good estimates on their behaviour up to the interaction point where the two potentials cross. This makes possible to compute the Wronskian of these four solutions at that point, and obtain in this way the condition of quantization that determines the resonances.

Then, a careful analysis of this condition leads to precise estimates on both the real part and the width of these resonances (see Theorem 2.1).

Let us mention that our methods still work for problems on $L^2(\mathbb{R}_+)$, with potentials $V_j(r)$ behaving like c_j/r^α in 0, with $c_j > 0$ and $0 \leq \alpha \leq 2$ (see Remark 8.8). Moreover, under an additional assumption on W , perturbations of size h^2 can be admitted, too, such as semiclassical pseudodifferential operators of order -2 , as it occurs after the Feshbach reduction in the Born-Oppenheimer reduction process ([19, 15, 20]): see Remark 2.2.

In the next section, we give the precise assumptions we work with, and we state our main result. Then, in Section 3.1, we construct fundamental solutions to the scalar operators both on the real negative half-line and on the positive half-line, and give estimates on them. These fundamental solutions are then used, in Section 4, to construct bounded solutions to the system in an iterative way, both on the negative half-line and on the positive half-line. In Section 5, these solutions and their derivatives are estimated more precisely at the crossing point, and, in Section 6, their Wronskian is computed and the quantization condition is written. In order to complete the proof, an analysis of this quantization condition is performed in Section 7, and additional informations are given concerning the resonant states. Finally, an appendix (Section 8) contains backgrounds on the Airy functions, some extensions of Yafaev's constructions for the scalar Schrödinger equation, and a list of formulas that may help the reader.

2. ASSUMPTIONS AND RESULTS

We consider a 2×2 Schrödinger operator of the type,

$$(2.1) \quad Pu = Eu, \quad P = \begin{pmatrix} P_1 & hW \\ hW^* & P_2 \end{pmatrix},$$

where D_x stands for $-i\frac{d}{dx}$, $P_j = h^2 D_x^2 + V_j(x)$ ($j = 1, 2$), $W = W(x, hD_x)$ is a semiclassical differential operator, and W^* is the formal adjoint of W .

We suppose the following conditions on the potentials $V_1(x), V_2(x)$ (see Figure 1) and on the interaction $W(x, hD_x)$:

Assumption (A1) $V_1(x), V_2(x)$ are real-valued analytic functions on \mathbb{R} , and extend to holomorphic functions in the complex domain,

$$\Gamma = \{x \in \mathbb{C}; |\operatorname{Im} x| < \delta_0 \langle \operatorname{Re} x \rangle\}$$

where $\delta_0 > 0$ is a constant, and $\langle t \rangle := (1 + |t|^2)^{1/2}$.

Assumption (A2) For $j = 1, 2$, V_j admits limits as $\operatorname{Re} x \rightarrow \pm\infty$ in Γ , and they satisfy,

$$\begin{aligned} \lim_{\substack{\operatorname{Re} x \rightarrow -\infty \\ x \in \Gamma}} V_1(x) &> 0; & \lim_{\substack{\operatorname{Re} x \rightarrow -\infty \\ x \in \Gamma}} V_2(x) &> 0; \\ \lim_{\substack{\operatorname{Re} x \rightarrow +\infty \\ x \in \Gamma}} V_1(x) &> 0; & \lim_{\substack{\operatorname{Re} x \rightarrow +\infty \\ x \in \Gamma}} V_2(x) &< 0. \end{aligned}$$

Assumption (A3) There exists a negative number $x^* < 0$ such that,

- $V_1 > 0$ and $V_2 > 0$ on $(-\infty, x^*)$;
- $V_1 < 0 < V_2$ on $(x^*, 0)$;
- $V_2 < 0 < V_1$ on $(0, +\infty)$,

and one has,

$$V_1'(x^*) =: -\tau_0 < 0, \quad V_1'(0) =: \tau_1 > 0, \quad V_2'(0) =: -\tau_2 < 0.$$

Assumption (A4) $W(x, hD_x)$ is a first order differential operator

$$W(x, hD_x) = r_0(x) + r_1(x)hD_x,$$

where r_0 and r_1 are bounded analytic functions on Γ , and $r_0(x)$ is real when x is real.

In this situation, the resonances of P can be defined, e.g., as the values $E \in \mathbb{C}$ such that the equation $Pu = Eu$ has a non trivial outgoing solution u , that is, a non identically vanishing solution such that, for some $\theta > 0$ sufficiently small, the function $x \mapsto u(xe^{i\theta})$ is in $L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$ (see, e.g., [1, 22]). Equivalently, the resonances are the eigenvalues of the operator P acting on $L^2(\mathbb{R}_\theta) \oplus L^2(\mathbb{R}_\theta)$, where \mathbb{R}_θ is a complex distortion of \mathbb{R} that coincides with $e^{i\theta}\mathbb{R}$ for $x \gg 1$ (see, e.g., [11]). We denote by $\text{Res}(P)$ the set of these resonances.

For $E \in \mathbb{C}$ small enough, we define the action,

$$\mathcal{A}(E) := \int_{x_1^*(E)}^{x_1(E)} \sqrt{E - V_1(t)} dt,$$

where $x_1^*(E)$ (respectively $x_1(E)$) is the unique solution of $V_1(x) = E$ close to x^* (respectively close to 0), and it is well-known that, in this situation, $\mathcal{A}(E)$ is an analytic function of E near 0.

We also fix $C_0 > 0$ arbitrarily large, and we plan to study the resonances of P lying in the set $\mathcal{D}_h(C_0)$ given by,

$$(2.2) \quad \mathcal{D}_h(C_0) := [-C_0 h^{2/3}, C_0 h^{2/3}] - i[0, C_0 h].$$

For $h > 0$ and $k \in \mathbb{Z}$, we set,

$$(2.3) \quad \lambda_k(h) := \frac{-2\mathcal{A}(0) + (2k+1)\pi h}{2\mathcal{A}'(0)h^{2/3}},$$

where $\mathcal{A}'(0) = \int_{x^*}^0 \frac{1}{2\sqrt{|V_1(x)|}} dx > 0$ is the first derivative of $\mathcal{A}(E)$ at 0. Then, our result is,

Theorem 2.1. *Under Assumptions (A1)-(A4), for $h > 0$ small enough, one has,*

$$\text{Res}(P) \cap \mathcal{D}_h(C_0) = \{E_k(h); k \in \mathbb{Z}\} \cap \mathcal{D}_h(C_0)$$

where the $E_k(h)$'s are complex numbers that satisfy,

$$(2.4) \quad \text{Re } E_k(h) = \lambda_k(h)h^{2/3} - \frac{\lambda_k(h)^2 \mathcal{A}''(0)}{2\mathcal{A}'(0)} h^{4/3} + \mathcal{O}(h^{5/3}),$$

$$(2.5) \quad \text{Im } E_k(h) = -\frac{2\pi^2 r_0(0)^2 (\mu_1(\lambda_k(h))^2 + \mu_2(\lambda_k(h))^2)}{\mathcal{A}'(0)} h^{5/3} + \mathcal{O}(h^2),$$

uniformly as $h \rightarrow 0_+$. Here, the functions μ_1 and μ_2 are defined by,

$$\begin{aligned}\mu_1(t) &:= \int_0^{+\infty} \text{Ai}(\tau_1^{-2/3}(\tau_1 y - t)) \text{Ai}(-\tau_2^{-2/3}(\tau_2 y + t)) dy; \\ \mu_2(t) &:= \int_0^{+\infty} \text{Ai}(\tau_2^{-2/3}(\tau_2 y - t)) \text{Ai}(-\tau_1^{-2/3}(\tau_1 y + t)) dy,\end{aligned}$$

where Ai stands for the usual Airy function.

Remark 2.1. One can always choose $k = k(h) \rightarrow +\infty$ in such a way that $\lambda_k(h) \rightarrow \rho_0$ as $h \rightarrow 0_+$, where $\rho_0 \in [-C_0, C_0]$ is fixed arbitrarily. In this case, (2.5) gives

$$\text{Im } E_k(h) = -\frac{2\pi^2 r_0(0)^2 (\mu_1(\rho_0)^2 + \mu_2(\rho_0)^2)}{\mathcal{A}'(0)} h^{5/3} + o(h^{5/3}).$$

In particular, if $r_0(0) \neq 0$ and $(\mu_1(\rho_0), \mu_2(\rho_0)) \neq (0, 0)$, then the result produces an equivalent of the width of the resonance as $h \rightarrow 0_+$, and it is of order $h^{5/3}$. Let us observe that one has,

$$\begin{aligned}\mu_1(t) + \mu_2(t) &= \int_{-\infty}^{+\infty} \text{Ai}(\tau_1^{-2/3}(\tau_1 y - t)) \text{Ai}(-\tau_2^{-2/3}(\tau_2 y + t)) dy \\ &= (\tau_1 + \tau_2)^{-1/3} \text{Ai}(-(\tau_1^{-1} + \tau_2^{-1})^{2/3} t),\end{aligned}$$

(where the last identity comes from an elementary computation involving the Fourier transform of Ai and interpreting $\mu_1 + \mu_2$ as a convolution of two Airy-type functions) and thus, the possible zeros of $\mu_1(\rho_0)^2 + \mu_2(\rho_0)^2$ are among those of the function $t \mapsto \text{Ai}(-(\tau_1^{-1} + \tau_2^{-1})^{2/3} t)$. In particular, they are necessarily positive. In the case where $\tau_1 = \tau_2$, this phenomenon does occur exactly at the zeros of $\text{Ai}(-2^{\frac{2}{3}} \tau_1^{-\frac{2}{3}} t)$, and for these special values of ρ_0 the result just says that $\text{Im } E_k(h)$ is $o(h^{5/3})$.

Remark 2.2. Under our assumptions, it can be proved that there exists an analytic distortion \tilde{P}_2 of P_2 such that, for $z \in \mathcal{D}_h(C_0)$, one has $\|(\tilde{P}_2 - z)^{-1}\|_{\mathcal{L}(L^2)} = \mathcal{O}(h^{-1})$, while the corresponding analytic distortion \tilde{P}_1 of P_1 satisfies $\|(\tilde{P}_1 - z)^{-1}\|_{\mathcal{L}(L^2)} = \mathcal{O}(\text{dis}(z, \sigma(P_1))^{-1})$. Using the ellipticity of \tilde{P}_1 and \tilde{P}_2 , and denoting by \tilde{W} and \tilde{W}^* the distorted operators obtained from W and W^* , we deduce that, if in addition $\min |z - \lambda_k(h)| \geq \delta h$ for some $\delta > 0$ constant, and if $\sup(|r_0| + |r_1|)$ is sufficiently small, then,

$$\|K(z)\| := \|h^2(\tilde{P}_2 - z)^{-1} \tilde{W}^*(\tilde{P}_1 - z)^{-1} \tilde{W}\| \leq 1/2.$$

Therefore, observing that the equation $(\tilde{P} - z)u = v$ is equivalent to $u_1 = (\tilde{P}_1 - z)^{-1}(v_1 - h\tilde{W}u_2)$ and $(1 - K(z))u_2 = (\tilde{P}_2 - z)^{-1}(v_2 - h\tilde{W}^*(\tilde{P}_1 - z)^{-1}v_1)$, we conclude that if the distance between $z \in \mathcal{D}_h(C_0)$ and the eigenvalues of \tilde{P} (that are the resonances of P) is at least of order h , then one has,

$$(2.6) \quad (\tilde{P} - z)^{-1} = \mathcal{O}(h^{-1}).$$

Since the resonances of P are separated from each other by a distance of order h , one can apply the standard perturbation theory and conclude that if \tilde{B} is a uniformly bounded operator on $L^2 \oplus L^2$, then the eigenvalues of $\tilde{P} + h^2 \tilde{B}$ in $\mathcal{D}_h(C_0)$ differ from those of \tilde{P} by $\mathcal{O}(h^2)$. In particular, in

this situation our result remains valid if we perturb P by a semiclassical pseudodifferential operator $h^2 B = h^2 b(x, hD_x)$ where b is a bounded analytic symbol in $\Gamma \times \Gamma$. This is typically what happens after the Feshbach reduction in the Born-Oppenheimer reduction process: see, e.g., [19, 15, 20].

3. FUNDAMENTAL SOLUTIONS

In order not to complicate too much the notation, we write the proof in the case $\tau_1 = \tau_2 = 1$ only, but it is clear that all our treatment can be performed with any other positive values of these parameters. At the end of the proof, we explain where the changes occur exactly.

From now on, we fix $\theta > 0$ small enough, and in the sequel we will use the following notation :

$$I_L := (-\infty, 0] = \mathbb{R}_- \quad ; \quad I_R^\theta := F_\theta([0, +\infty)) = F_\theta(\mathbb{R}_+),$$

where $F_\theta(x) := x + i\theta f(x)$, with $f \in C^\infty(\mathbb{R}_+, \mathbb{R}_+)$, $f(x) = x$ for x large enough, $f(x) = 0$ for $x \in [0, x_\infty]$ for some $x_\infty > 0$, and f is chosen in such a way that, for any $x \geq x_\infty$, one has,

$$(3.1) \quad \operatorname{Im} \int_{x_\infty}^{F_\theta(x)} \sqrt{E - V_2(t)} dt \geq -Ch,$$

for some positive constant C , where the first integral is taken along I_R^θ (observe that, for $E \in \mathcal{D}_h(C_0)$ and $C > 0$ sufficiently large, one always has $\operatorname{Im} \int_{Ch^{\frac{2}{3}}}^{x_\infty} \sqrt{E - V_2(t)} dt = \mathcal{O}(h)$). Performing a Taylor expansion of this quantity as $\theta \rightarrow 0_+$, and using the fact that (thanks to Cauchy estimates on a complex sector around the positive real axis), for any $k \geq 1$, one has $t^k V_2^{(k)}(t) \rightarrow 0$ as $t \rightarrow +\infty$, we see that it is sufficient to choose x_∞ sufficiently large and that f satisfies,

$$f'(t) \geq \delta(t^{-1}f(t) + t^{-3}f(t)^3)$$

for some $\delta > 0$ constant. By taking f strictly increasing on $[x_\infty, +\infty)$, we see that the only possible problem is near x_∞ , but there one can take for instance $f(s) := e^{-1/(s-x_\infty)^2}$.

3.1. Fundamental solutions on I_L . On $I_L := (-\infty, 0]$, and for $E \in \mathcal{D}_h(C_0)$ and $j = 1, 2$, let $u_{j,L}^\pm$ be the solutions to $(P_j - E)u = 0$ constructed in Appendix 8.2 (in particular, $u_{j,L}^-$ decays exponentially at $-\infty$, while $u_{j,L}^+$ grows exponentially). Then, the Wronskian $\mathcal{W}[u_{j,L}^-, u_{j,L}^+]$ is independent of the variable x and satisfies

$$(3.2) \quad \mathcal{W}[u_{j,L}^-, u_{j,L}^+] = \frac{-2}{\pi h^{\frac{2}{3}}}(1 + \mathcal{O}(h)) \quad (h \rightarrow 0).$$

For any $k \geq 0$ integer, we set,

$$C_b^k(I_L) := \{u : I_L \rightarrow \mathbb{C} \text{ of class } C^k ; \sum_{0 \leq j \leq k} \sup_{x \in I_L} |u^{(j)}(x)| < +\infty\},$$

equipped with the norm $\|u\|_{C_b^k(I_L)} := \sum_{0 \leq j \leq k} \sup_{I_L} |u^{(j)}|$, and we define a fundamental solution

$$K_{j,L} : C_b^0(I_L) \rightarrow C_b^2(I_L) \quad (j = 1, 2),$$

of $P_j - E$ on I_L by setting, for $v \in C_b^0(I_L)$,

$$(3.3) \quad K_{j,L}[v](x) := \frac{u_{j,L}^+(x)}{h^2 \mathcal{W}[u_{j,L}^+, u_{j,L}^-]} \int_{-\infty}^x u_{j,L}^-(t) v(t) dt + \frac{u_{j,L}^-(x)}{h^2 \mathcal{W}[u_{j,L}^+, u_{j,L}^-]} \int_x^0 u_{j,L}^+(t) v(t) dt.$$

Then, $K_{j,L}$ satisfies,

$$(P_j - E)K_{j,L} = \mathbf{1},$$

and, because of the form of the operator W , an integration by parts shows that we also have,

$$K_{j,L}W, K_{j,L}W^* : C_b^0(I_L) \rightarrow C_b^0(I_L) \quad (j = 1, 2).$$

In view of the construction of solutions to the system, we prove,

Proposition 3.1. *As h goes to 0_+ , one has,*

$$(3.4) \quad \|hK_{2,L}W^*\|_{\mathcal{L}(C_b^0(I_L))} = \mathcal{O}(h^{\frac{1}{3}});$$

$$(3.5) \quad \|h^2K_{1,L}WK_{2,L}W^*\|_{\mathcal{L}(C_b^0(I_L))} = \mathcal{O}(h^{\frac{2}{3}}).$$

Proof. For $j = 1, 2$, we set,

$$(3.6) \quad \begin{aligned} \tilde{u}_{j,L}^\pm(x) &:= \max\{|u_{j,L}^\pm(x)|, |h\partial_x u_{j,L}^\pm(x)|\}; \\ U_j(x, t) &:= \tilde{u}_{j,L}^+(x)\tilde{u}_{j,L}^-(t)\mathbf{1}_{\{t < x\}} + \tilde{u}_{j,L}^-(x)\tilde{u}_{j,L}^+(t)\mathbf{1}_{\{t > x\}} = U_j(t, x). \end{aligned}$$

Thanks to our choice of $K_{j,L}$, and doing an integration by parts, we see that we have,

$$(3.7) \quad \begin{aligned} |hK_{1,L}Wv(x)| &= \mathcal{O}(h^{-\frac{1}{3}}) \left(\int_{-\infty}^0 U_1(x, t)|v(t)|dt + hU_1(x, 0)|v(0)| \right); \\ |hK_{2,L}W^*v(x)| &= \mathcal{O}(h^{-\frac{1}{3}}) \left(\int_{-\infty}^0 U_2(x, t)|v(t)|dt + hU_2(x, 0)|v(0)| \right). \end{aligned}$$

In particular,

$$(3.8) \quad \|hK_{2,L}W^*\| = \mathcal{O}(h^{-\frac{1}{3}}) \sup_{x \in I_L} \int_{-\infty}^0 U_2(x, t)dt + \mathcal{O}(h^{\frac{2}{3}}) \sup_{x \in I_L} U_2(x, 0).$$

Moreover, using the asymptotics of $u_{2,L}^\pm$ and $h\partial_x u_{2,L}^\pm$ on I_L , and fixing some constant $C_1 > 0$ sufficiently large, we obtain,

- If $x, t \leq -C_1 h^{\frac{2}{3}}$, then,

$$(3.9) \quad U_2(x, t) = \mathcal{O}(h^{\frac{1}{3}}) \frac{e^{-|\operatorname{Re} \int_t^x (V_2 - E)^{1/2}|/h}}{|(V_2(x) - E)(V_2(t) - E)|^{\frac{1}{4}}};$$

- If $t \leq -C_1 h^{\frac{2}{3}} \leq x \leq 0$, then,

$$(3.10) \quad U_2(x, t) = \mathcal{O}(h^{\frac{1}{6}}) \frac{e^{-|\operatorname{Re} \int_0^t (V_2 - E)^{1/2}|/h}}{|(V_2(t) - E)|^{\frac{1}{4}}};$$

- If $x, t \in [-C_1 h^{\frac{2}{3}}, 0]$, then $U_2(x, t) = \mathcal{O}(1)$.

Hence $U_2(x, t) = \mathcal{O}(1)$ uniformly, and when $x \leq -\delta$ with $\delta > 0$ constant, there exists a positive constant α such that,

$$\int_{-\infty}^0 U_2(x, t) dt = \mathcal{O}(h^{\frac{1}{3}}) \int_{-\infty}^{-\delta/2} e^{-\alpha|x-t|/h} dt + \mathcal{O}(e^{-\alpha/h}) = \mathcal{O}(h^{\frac{4}{3}}).$$

On the other hand, if δ is chosen sufficiently small and $x \in [-\delta, -C_1 h^{\frac{2}{3}}]$, then, there exists a (different) positive constant α such that,

$$\begin{aligned} \int_{-\infty}^0 U_2(x, t) dt &= \int_{-2\delta}^{-C_1 h^{\frac{2}{3}}} U_2(x, t) dt + \mathcal{O}(h^{\frac{2}{3}}) \\ &= \mathcal{O}(h^{\frac{1}{3}} |x|^{-\frac{1}{4}}) \int_{C_1 h^{\frac{2}{3}}}^{2\delta} \frac{e^{-\alpha|t^{\frac{3}{2}} - |x|^{\frac{3}{2}}|/h}}{t^{\frac{1}{4}}} dt + \mathcal{O}(h^{\frac{2}{3}}). \end{aligned}$$

Setting $t = (hs)^{\frac{2}{3}}$ in the integral, we obtain,

$$\int_{-\infty}^0 U_2(x, t) dt = \mathcal{O}(h^{\frac{1}{3}} |x|^{-\frac{1}{4}} h^{\frac{2}{3} - \frac{1}{6}}) \int_1^{\infty} \frac{e^{-\alpha|s - h^{-1}|x|^{\frac{3}{2}}|}}{\sqrt{s}} ds + \mathcal{O}(h^{\frac{2}{3}}) = \mathcal{O}(h^{\frac{2}{3}}).$$

Finally, when $x \in [-C_1 h^{\frac{2}{3}}, 0]$, we have,

$$\begin{aligned} \int_{-\infty}^0 U_2(x, t) dt &= \int_{-\delta}^{-C_1 h^{\frac{2}{3}}} U_2(x, t) dt + \mathcal{O}(h^{\frac{2}{3}}) \\ &= \mathcal{O}(h^{\frac{1}{6}}) \int_{C_1 h^{\frac{2}{3}}}^{\delta} \frac{e^{-\alpha t^{\frac{3}{2}}/h}}{t^{\frac{1}{4}}} dt + \mathcal{O}(h^{\frac{2}{3}}) = \mathcal{O}(h^{\frac{2}{3}}). \end{aligned}$$

Thus, we have proved,

$$(3.11) \quad \sup_{x \leq 0} \int_{-\infty}^0 U_2(x, t) dt = \mathcal{O}(h^{\frac{2}{3}}),$$

and, by (3.8) (and the fact that $U_2 = \mathcal{O}(1)$), (3.4) follows.

Now, let us prove the estimate for $M_L := h^2 K_{1,L} W K_{2,L} W^*$. We see from the definition of $K_{1,L}$ and from (3.7) that we have,

$$\begin{aligned} |M_L v(x)| &\leq C h^{-\frac{2}{3}} \int_{-\infty}^0 \int_{-\infty}^0 U_1(x, t) U_2(t, s) |v(s)| ds dt \\ &\quad + C h^{\frac{1}{3}} \int_{-\infty}^0 U_1(x, t) U_2(t, 0) |v(0)| dt \\ &\quad + C h^{\frac{1}{3}} U_1(x, 0) \int_{-\infty}^0 U_2(0, t) |v(t)| dt \\ &\quad + C h^{\frac{4}{3}} U_1(x, 0) U_2(0, 0) |v(0)|. \end{aligned} \tag{3.12}$$

Using (3.11) and the fact that $U_j = \mathcal{O}(1)$ uniformly ($j = 1, 2$), we see that the last three terms are $\mathcal{O}(h) \sup_{I_L} |v|$ (observe that $U_j(t, x) = U_j(x, t)$ for all x, t).

In order to estimate the integral, we use the following properties of U_1 : For any $\delta > 0$ small enough, there exists $\alpha > 0$ constant, such that,

- If $x, t \leq x^* - \delta$, then,

$$U_1(x, t) = \mathcal{O}(h^{\frac{1}{3}}) e^{-\alpha|t-x|/h};$$

- If $t \leq x^* - 2\delta$ and $x \in [x^* - \delta, 0]$, then,

$$U_1(x, t) = \mathcal{O}(h^{\frac{1}{6}} e^{-\alpha/h});$$

- If $x \in [x^* - 4\delta, 0]$ and $t \in [-\delta, -C_1 h^{\frac{2}{3}}]$, then $U_1(x, t) = \mathcal{O}(h^{\frac{1}{6}} |t|^{-\frac{1}{4}})$;
- If $x \in [x^* - 4\delta, 0]$ and $t \in [-C_1 h^{\frac{2}{3}}, 0] \cup [x^* - 4\delta, -\delta]$, then $U_1(x, t) = \mathcal{O}(1)$.

Moreover, by the properties of U_2 , we also know that any part of the integral corresponding to $|t - s| \geq \delta$ with $\delta > 0$ constant is exponentially small.

We first consider the case $x \in (-\infty, x^* - 2\delta]$ for some small positive constant δ .

Then, we see that there exists a constant $\alpha > 0$ such that,

$$\begin{aligned} \iint_{-\infty}^0 U_1(x, t) U_2(t, s) dt ds &= \mathcal{O}(h^{\frac{2}{3}}) \int_{-\infty}^{x^* - \delta} dt \int_{-\infty}^{x^* - \delta/2} e^{-\alpha(|t-x|+|s-t|)/h} ds \\ &\quad + \mathcal{O}(e^{-\alpha/h}) \\ &= \mathcal{O}(h^{2+\frac{2}{3}}). \end{aligned}$$

Now, when $x \in [x^* - 2\delta, 0]$, and still denoting by α every new positive constant that may appear, we have,

$$\iint_{-\infty}^0 U_1(x, t) U_2(t, s) dt ds = \int_{x^* - 3\delta}^0 dt \int_{x^* - 4\delta}^0 U_1(x, t) U_2(t, s) ds + \mathcal{O}(e^{-\alpha/h}),$$

and,

$$\begin{aligned} &\int_{x^* - 3\delta}^0 dt \int_{x^* - 4\delta}^0 U_1(x, t) U_2(t, s) ds \\ &= \mathcal{O}(h^{\frac{1}{3}}) \int_{x^* - 3\delta}^{-\delta} dt \int_{x^* - 4\delta}^{-\delta/2} e^{-\alpha|t-s|/h} ds + \mathcal{O}(e^{-\alpha/h}) \\ &\quad + \mathcal{O}(h^{\frac{1}{2}}) \int_{-\delta}^{-C_1 h^{\frac{2}{3}}} dt \int_{-2\delta}^{-C_1 h^{\frac{2}{3}}} \frac{e^{-\alpha(|t|^{\frac{3}{2}} - |s|^{\frac{3}{2}})/h}}{|t|^{\frac{1}{2}} |s|^{\frac{1}{4}}} ds \\ &\quad + \mathcal{O}(h^{\frac{1}{6}}) \int_{-\delta}^{-C_1 h^{\frac{2}{3}}} dt \int_{-C_1 h^{\frac{2}{3}}}^0 \frac{e^{-\alpha|t|^{\frac{3}{2}}/h}}{|t|^{\frac{1}{4}}} ds \\ &\quad + \mathcal{O}(h^{\frac{1}{6}}) \int_{-C_1 h^{\frac{2}{3}}}^0 dt \int_{-\delta}^{-C_1 h^{\frac{2}{3}}} \frac{e^{-\alpha|s|^{\frac{3}{2}}/h}}{|s|^{\frac{1}{4}}} ds + \mathcal{O}(h^{\frac{4}{3}}). \end{aligned}$$

Hence,

(3.13)

$$\begin{aligned} \int_{x^*-3\delta}^0 dt \int_{x^*-4\delta}^0 U_1(x, t) U_2(t, s) ds &= \mathcal{O}(h^{\frac{1}{2}}) \int_{C_1 h^{\frac{2}{3}}}^{\delta} dt \int_{C_1 h^{\frac{2}{3}}}^{2\delta} \frac{e^{-\alpha|t^{\frac{3}{2}}-s^{\frac{3}{2}}|/h}}{t^{\frac{1}{2}} s^{\frac{1}{4}}} ds \\ &\quad + \mathcal{O}(h^{\frac{5}{6}}) \int_{C_1 h^{\frac{2}{3}}}^{\delta} \frac{e^{-\alpha t^{\frac{3}{2}}/h}}{t^{\frac{1}{4}}} dt + \mathcal{O}(h^{\frac{4}{3}}). \end{aligned}$$

For the first term, the change of variables $(t, s) \mapsto (t^{2/3}, s^{2/3})$ gives,

$$\int_{C_1 h^{\frac{2}{3}}}^{\delta} dt \int_{C_1 h^{\frac{2}{3}}}^{2\delta} \frac{e^{-\alpha|t^{\frac{3}{2}}-s^{\frac{3}{2}}|/h}}{t^{\frac{1}{2}} s^{\frac{1}{4}}} ds = \mathcal{O}(1) \iint_{C_2 h}^{\delta'} \frac{e^{-\alpha|t-s|/h}}{t^{2/3} s^{1/2}} dt ds,$$

with $C_2 := C_1^{2/3}$ and $\delta' := (2\delta)^{2/3}$. Dividing this integral in two parts, depending whether $t \leq s$ or $s \leq t$, and first integrating with respect to the larger of the two variables, we obtain,

$$\begin{aligned} (3.14) \quad \int_{C_1 h^{\frac{2}{3}}}^{\delta} dt \int_{C_1 h^{\frac{2}{3}}}^{2\delta} \frac{e^{-\alpha|t^{\frac{3}{2}}-s^{\frac{3}{2}}|/h}}{t^{\frac{1}{2}} s^{\frac{1}{4}}} ds &= \mathcal{O}(1) \int_{C_2 h}^{\delta'} dt \frac{e^{\alpha t/h}}{t^{7/6}} \int_t^{\delta'} e^{-\alpha s/h} ds \\ &= \mathcal{O}(h^{5/6}). \end{aligned}$$

Moreover, a simple change of variable gives,

$$\int_{C_1 h^{\frac{2}{3}}}^{\delta} \frac{e^{-\alpha t^{\frac{3}{2}}/h}}{t^{\frac{1}{4}}} dt = \mathcal{O}(h^{\frac{1}{2}}).$$

Inserting into (3.13), we deduce that, for $x \in [x^* - 2\delta, 0]$, we have,

$$(3.15) \quad \iint_{-\infty}^0 U_1(x, t) U_2(t, s) dt ds = \mathcal{O}(h^{4/3}).$$

Finally, going back to (3.12), we conclude (3.5). \square

3.2. Fundamental solutions on I_R^θ . On \mathbb{R}_+ , let $u_{1,R}^\pm$ (resp. $u_{2,L}^\pm$) be the solutions to $(P_1 - E)u = 0$ (resp. $(P_2 - E)u = 0$) constructed in Appendix 8.2. Setting,

$$(3.16) \quad u_{2,R}^\pm := 2^{\pm\frac{1}{2}} e^{i\frac{\pi}{4}} \left(\frac{1}{2} a_2^- u_{2,L}^- \pm i a_2^+ u_{2,L}^+ \right)$$

by Proposition 8.5 we have,

$$u_{2,R}^\pm(x) \sim (1 + \mathcal{O}(h)) \frac{h^{\frac{1}{6}} e^{i\frac{\pi}{4}}}{\sqrt{2\pi}} (E - V_2(x))^{-1/4} e^{\mp i \int_0^x \sqrt{E - V_2(t)} dt/h} \quad (x \rightarrow +\infty).$$

Then, all these solutions can be extended as holomorphic functions in a complex sector around \mathbb{R}_+ , and in particular (thanks to (3.1)), $u_{j,R}^-$ ($j = 1, 2$) remains uniformly bounded on I_R^θ , and exponentially decaying at infinity along I_R^θ . Moreover, the Wronskians $\mathcal{W}[u_{j,R}^-, u_{j,R}^+]$ are independent of the variable x and satisfy,

$$(3.17) \quad \mathcal{W}[u_{j,R}^-, u_{j,R}^+] = \frac{2}{\pi h^{\frac{2}{3}}} (1 + \mathcal{O}(h)) \quad (h \rightarrow 0).$$

We define a fundamental solution of $P_j - E$ on I_R^θ as,

$$(3.18) \quad K_{j,R}[v](x) := \frac{u_{j,R}^-(x)}{h^2 \mathcal{W}[u_{j,R}^-, u_{j,R}^+]} \int_0^x u_{j,R}^+(t) v(t) dt + \frac{u_{j,R}^+(x)}{h^2 \mathcal{W}[u_{j,R}^-, u_{j,R}^+]} \int_x^{+\infty} u_{j,R}^-(t) v(t) dt,$$

where v is in the space $C_b^0(I_R^\theta)$ of bounded continuous functions on I_R^θ , and the integrals run over I_R^θ .

Then, using the semiclassical asymptotic behaviour of $u_{j,R}^\pm$ on I_R^θ , one can prove exactly as for (3.4)-(3.5) (x_∞ playing the role of x^*) that we have,

Proposition 3.2. *One has,*

$$(3.19) \quad \| h K_{1,R} W \|_{\mathcal{L}(C_b^0(I_R^\theta))} = \mathcal{O}(h^{\frac{1}{3}});$$

$$(3.20) \quad \| h^2 K_{2,R} W^* K_{1,R} W \|_{\mathcal{L}(C_b^0(I_R^\theta))} = \mathcal{O}(h^{\frac{2}{3}}),$$

uniformly as h goes to 0_+ .

4. SOLUTIONS ON I_L AND I_R^θ

In this section, we use the previous constructions of fundamental solutions in order to construct solutions to the system (2.1) in I_L and I_R^θ .

We first consider the interval I_L . We set,

$$w_{1,L}^0 := \begin{pmatrix} u_{1,L}^- \\ 0 \end{pmatrix} \quad ; \quad w_{2,L}^0 := \begin{pmatrix} 0 \\ u_{2,L}^- \end{pmatrix},$$

and we look for solutions $u := \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$ to (2.1) in I_L , that are close to $w_{1,L}^0$ or $w_{2,L}^0$ as $h \rightarrow 0$. We rewrite (2.1) as,

$$\begin{cases} (P_1 - E)u_1 = -hWu_2; \\ (P_2 - E)u_2 = -hW^*u_1. \end{cases}$$

Assuming that u_1 is in $C_b^0(I_L)$, we set $u_2 = -hK_{2,L}W^*u_1$, so that the system reduces to,

$$(P_1 - E)u_1 = h^2WK_{2,L}W^*u_1,$$

and a solution will be given by any $u_1 \in C_b^0(I_L)$ such that,

$$u_1 = u_{1,L}^- + h^2K_{1,L}WK_{2,L}W^*u_1.$$

Now, by Proposition 3.1, the operator $M_L := h^2K_{1,L}WK_{2,L}W^*$ is $\mathcal{O}(h^{\frac{2}{3}})$ when acting on $C_b^0(I_L)$. By construction, we also know that $u_{1,L}^-$ is in $C_b^0(I_L)$. Therefore, we can define,

$$(4.1) \quad w_{1,L} := \begin{pmatrix} \sum_{j \geq 0} M_L^j u_{1,L}^- \\ -hK_{2,L}W^* \sum_{j \geq 0} M_L^j u_{1,L}^- \end{pmatrix} \in C_b^0(I_L)^2,$$

and $w_{1,L}$ is solution to (2.1) in I_L , with $w_{1,L} \rightarrow w_{1,L}^0$ as $h \rightarrow 0_+$. In a similar way, we can define,

$$(4.2) \quad w_{2,L} := \begin{pmatrix} -\sum_{j \geq 0} M_L^j(hK_{1,L}Wu_{2,L}^-) \\ u_{2,L}^- + hK_{2,L}W^* \sum_{j \geq 0} M_L^j(hK_{1,L}Wu_{2,L}^-) \end{pmatrix} \in C_b^0(I_L)^2,$$

that is solution to (2.1) in I_L , with $w_{2,L} \rightarrow w_{2,L}^0$ as $h \rightarrow 0_+$.

Remark 4.1. The standard WKB method (see, e.g., [7, 23]) gives us asymptotic expansions for $u_{j,L}^-$ ($j = 1, 2$) inside $(x^*, 0)$, of the form,

$$(4.3) \quad \begin{aligned} u_{1,L}^- &\sim \frac{2h^{\frac{1}{6}}}{\sqrt{\pi}}(E - V_1(x))^{-1/4} \sin\left(\frac{\mathcal{A}(E) + \nu_1(x)}{h} + \frac{\pi}{4}\right) \left(1 + \sum_{k \geq 1} a_{1,k}(x)h^k\right) \\ &\quad + \frac{2h^{\frac{1}{6}}}{\sqrt{\pi}}(E - V_1(x))^{-1/4} \cos\left(\frac{\mathcal{A}(E) + \nu_1(x)}{h} + \frac{\pi}{4}\right) \sum_{k \geq 1} b_{1,k}(x)h^k; \\ u_{2,L}^- &\sim \frac{h^{\frac{1}{6}}}{\sqrt{\pi}}(V_2(x) - E)^{-1/4} e^{-\frac{1}{h} \int_x^{x_2(E)} \sqrt{V_2(t) - E} dt} \left(1 + \sum_{k \geq 1} a_{2,k}(x)h^k\right), \end{aligned}$$

where $x_2(E)$ is the unique solution of $V_2(x) = E$ close to 0, $\nu_1(x) := \int_{x_1(E)}^x \sqrt{E - V_1(t)} dt$.

Now, on I_R^θ , a similar construction can be done by using Proposition 3.2, and by starting from the solutions $u_{j,R}^-$ ($j = 1, 2$) to $(P_j - E)u_{j,R}^- = 0$ on I_R^θ . Setting $M_R := h^2 K_{2,R}W^* K_{1,R}W$, by Proposition 3.2 we have $\|M_R\| = \mathcal{O}(h^{\frac{2}{3}})$, and thus, defining,

$$(4.4) \quad w_{1,R} := \begin{pmatrix} u_{1,R}^- + hK_{1,R}W \sum_{j \geq 0} M_R^j(hK_{2,R}W^*u_{1,R}^-) \\ -\sum_{j \geq 0} M_R^j(hK_{2,R}W^*u_{1,R}^-) \end{pmatrix} \in C_b^0(I_R^\theta)^2;$$

$$(4.5) \quad w_{2,R} := \begin{pmatrix} -hK_{1,R}W \sum_{j \geq 0} M_R^j u_{2,R}^- \\ \sum_{j \geq 0} M_R^j u_{2,R}^- \end{pmatrix} \in C_b^0(I_R^\theta)^2,$$

we see that they are both solutions to (2.1) on I_R^θ , and they respectively approach $w_{1,R}^0 := \begin{pmatrix} u_{1,R}^- \\ 0 \end{pmatrix}$ and $w_{2,R}^0 := \begin{pmatrix} 0 \\ u_{2,R}^- \end{pmatrix}$, as $h \rightarrow 0_+$.

Remark 4.2. Still by the standard WKB method, we have asymptotic expansions for $u_{j,R}^-$ ($j = 1, 2$) inside $(0, +\infty)$, of the form,

$$(4.6) \quad \begin{aligned} u_{1,R}^- &\sim \frac{\pi^{\frac{1}{2}} h^{\frac{1}{6}}}{2}(V_1(x) - E)^{-1/4} e^{-\frac{1}{h} \int_{x_1(E)}^x \sqrt{V_1(t) - E} dt} \left(1 + \sum_{k \geq 1} b_{1,k}(x)h^k\right); \\ u_{2,R}^- &\sim \frac{\pi^{\frac{1}{2}} h^{\frac{1}{6}}}{2}(E - V_2(x))^{-1/4} e^{\frac{i}{h} \int_{x_2(E)}^x \sqrt{E - V_2(t)} dt} \left(1 + \sum_{k \geq 1} b_{2,k}(x)h^k\right). \end{aligned}$$

The solutions we have just constructed are not only bounded, and actually we have,

Proposition 4.1. *The solutions $w_{j,L}$ given by (4.1)-(4.2), and $w_{j,R}$ given by (4.4)-(4.5) ($j = 1, 2$) satisfy,*

$$w_{j,L} \in L^2(I_L) \oplus L^2(I_L) \quad ; \quad w_{j,R} \in L^2(I_R^\theta) \oplus L^2(I_R^\theta).$$

Proof. It is sufficient to prove that, for any $N \geq 1$, one has $w_{j,S} = \mathcal{O}(\langle x \rangle^{-N})$ as $|x| \rightarrow \infty$ (on I_L or I_R^θ , depending if $S = L$ or $S = R$). But thanks to the exponential decay of $U_j(x, t)$ ($j = 1, 2$) as $|x - t| \rightarrow \infty$, $|x| \gg 1$, we immediately see that (3.11) and (3.15) remain valid with $U_j(x, t)$ replaced by $\langle x \rangle^N U_j(x, t) \langle t \rangle^{-N}$. As a consequence, the estimates of Proposition 3.1 extend to the operators $\langle x \rangle^N h K_{2,L} W^* \langle x \rangle^{-N}$ and $\langle x \rangle^N h^2 K_{1,L} W K_{2,L} W^* \langle x \rangle^{-N}$, and since $\langle x \rangle^N u_{j,L}^- \in C_b^0(I_L)$ ($j = 1, 2$), the result for $w_{j,L}$ follows. The same arguments apply in I_R^θ , and the result for $w_{j,R}$ follows, too. \square

Now, by general theory on systems of ordinary differential equations, we know that the space of solutions to (2.1) that are L^2 in I_L (resp. in I_R^θ) is at most two-dimensional. As a consequence, the previous proposition implies,

Proposition 4.2. *E is a resonance if and only if the four solutions $w_{1,L}$, $w_{2,L}$, $w_{1,R}$ and $w_{2,R}$ are linearly dependent.*

5. ESTIMATES AT THE CROSSING POINT

In this section, we investigate the asymptotic behaviours of $w_{j,L}(x)$, $w_{j,R}(x)$, and their first derivative at $x = 0$.

We first prove,

Proposition 5.1. *Let $x_0 \in (x^*, 0)$. Then, for $x \in [x_0, 0]$, one has,*

$$(5.1) \quad u_{1,L}^\pm = a_\pm u_{1,R}^- + b_\pm u_{1,R}^+,$$

with,

$$\begin{aligned} a_- &= \sin \frac{\mathcal{A}(E)}{h} + \mathcal{O}(h) \quad ; \quad b_- = 2 \cos \frac{\mathcal{A}(E)}{h} + \mathcal{O}(h); \\ a_+ &= \frac{1}{2} \cos \frac{\mathcal{A}(E)}{h} + \mathcal{O}(h) \quad ; \quad b_+ = -\sin \frac{\mathcal{A}(E)}{h} + \mathcal{O}(h), \end{aligned}$$

uniformly as $h \rightarrow 0_+$.

Proof. Since $(u_{1,R}^-, u_{1,R}^+)$ is a basis of solutions to $(P_1 - E)u = 0$, we know that (5.1) is verified with,

$$a_- = \frac{\mathcal{W}(u_{1,L}^-, u_{1,R}^+)}{\mathcal{W}(u_{1,R}^-, u_{1,R}^+)} \quad ; \quad b_- = \frac{\mathcal{W}(u_{1,R}^-, u_{1,L}^-)}{\mathcal{W}(u_{1,R}^-, u_{1,R}^+)}.$$

We compute these Wronskians at some arbitrary point in $x \in (x^*, 0)$, by using formula (4.3), Proposition 8.2 and (3.17). By (4.3), we have,

$$\begin{aligned} u_{1,L}^-(x) &= \frac{2h^{\frac{1}{6}}}{\sqrt{\pi}(E - V_1(x))^{\frac{1}{4}}} \cos \left(\frac{\mathcal{A}(E) + \nu_1(x)}{h} - \frac{\pi}{4} \right) + \mathcal{O}(h^{\frac{7}{6}}); \\ (u_{1,L}^-)'(x) &= -\frac{2h^{\frac{1}{6}}(E - V_1(x))^{\frac{1}{4}}}{h\sqrt{\pi}} \sin \left(\frac{\mathcal{A}(E) + \nu_1(x)}{h} - \frac{\pi}{4} \right) + \mathcal{O}(h^{\frac{1}{6}}). \end{aligned}$$

Therefore, using Proposition 8.2 and (8.12), we obtain,

$$\begin{aligned} \mathcal{W}(u_{1,L}^-, u_{1,R}^+) &= \frac{2h^{-\frac{1}{2}}(\xi_1')^{\frac{1}{2}}}{\sqrt{\pi}(E - V_1)^{\frac{1}{4}}} \cos\left(\frac{\mathcal{A}(E) + \nu_1(x)}{h} - \frac{\pi}{4}\right) \text{Bi}'(h^{-\frac{2}{3}}\xi_1) \\ &\quad + \frac{2h^{-\frac{5}{6}}(E - V_1)^{\frac{1}{4}}}{\sqrt{\pi}(\xi_1')^{\frac{1}{2}}} \sin\left(\frac{\mathcal{A}(E) + \nu_1(x)}{h} - \frac{\pi}{4}\right) \text{Bi}(h^{-\frac{2}{3}}\xi_1) \\ &\quad + \mathcal{O}(h^{\frac{1}{3}}). \end{aligned}$$

Then, using the asymptotic behaviour of Bi and Bi' at $-\infty$, and observing that one has the identity $\frac{2}{3}(-\xi_1)^{\frac{3}{2}} = -\nu_1$ (so that $(\xi_1')^{\frac{1}{2}} = (E - V_1)^{1/4}(-\xi_1)^{-1/4}$), this gives,

$$\begin{aligned} W(u_{1,L}^-, u_{1,R}^+) &= \frac{2h^{-\frac{2}{3}}}{\pi} \cos\left(\frac{\mathcal{A}(E) + \nu_1(x)}{h} - \frac{\pi}{4}\right) \cos\left(\frac{\nu_1}{h} + \frac{\pi}{4}\right) \\ &\quad + \frac{2h^{-\frac{2}{3}}}{\pi} \sin\left(\frac{\mathcal{A}(E) + \nu_1(x)}{h} - \frac{\pi}{4}\right) \sin\left(\frac{\nu_1}{h} + \frac{\pi}{4}\right) + \mathcal{O}(h^{\frac{1}{3}}) \\ &= \frac{2h^{-\frac{2}{3}}}{\pi} \sin \frac{\mathcal{A}(E)}{h} + \mathcal{O}(h^{\frac{1}{3}}), \end{aligned}$$

and thus, by (3.17),

$$a_- = \sin \frac{\mathcal{A}(E)}{h} + \mathcal{O}(h).$$

The same arguments hold for b_- , a_+ , b_+ , and the result follows. \square

From now on, we set,

$$(5.2) \quad \tilde{\partial} := \varepsilon^2 \partial_x,$$

and we will use this operator in all the Wronskians that will appear (instead of the usual derivative), denoting them by $\tilde{\mathcal{W}}$ instead of \mathcal{W} .

Proposition 5.2. *For $j = 1, 2$ and $S = L, R$, there exist complex numbers $\alpha_{j,S}, \beta_{j,S}$, such that,*

$$(5.3) \quad \begin{aligned} w_{1,S}(0) &= \begin{bmatrix} u_{1,S}^-(0) + \beta_{1,S} u_{1,S}^+(0) \\ \alpha_{1,S} u_{2,S}^+(0) \end{bmatrix} + \mathcal{O}(h); \\ \tilde{w}_{1,S}(0) &= \begin{bmatrix} \tilde{\partial} u_{1,S}^-(0) + \beta_{1,S} \tilde{\partial} u_{1,S}^+(0) \\ \alpha_{1,S} \tilde{\partial} u_{2,S}^+(0) \end{bmatrix} + \mathcal{O}(h), \end{aligned}$$

$$(5.4) \quad \begin{aligned} w_{2,S}(0) &= \begin{bmatrix} \alpha_{2,S} u_{1,S}^+(0) \\ u_{2,S}^-(0) + \beta_{2,S} u_{2,S}^+(0) \end{bmatrix} + \mathcal{O}(h); \\ \tilde{w}_{2,S}(0) &= \begin{bmatrix} \alpha_{2,S} \tilde{\partial} u_{1,S}^+(0) \\ \tilde{\partial} u_{2,S}^-(0) + \beta_{2,S} \tilde{\partial} u_{2,S}^+(0) \end{bmatrix} + \mathcal{O}(h), \end{aligned}$$

uniformly as $h \rightarrow 0_+$.

Proof. We prove (5.3) and (5.4) in the case $S = L$ only (the case $S = R$ being similar). We start with $j = 1$. By (4.1), we have,

$$(5.5) \quad w_{1,L} := \begin{pmatrix} u_{1,L}^- + hK_{1,L}W r_{1,L} \\ -r_{1,L} \end{pmatrix} + \mathcal{O}(h),$$

with,

$$r_{1,L} := hK_{2,L}W^*u_{1,L}^-.$$

In particular, using the expression (3.3) of $K_{2,L}$, we find

$$r_{1,L}(0) = -\alpha_{1,L}u_{2,L}^+(0),$$

with,

$$(5.6) \quad \alpha_{1,L} := \frac{-1}{h\mathcal{W}(u_{2,L}^+, u_{2,L}^-)} \int_{-\infty}^0 u_{2,L}^-(t)(W^*u_{1,L}^-)(t)dt.$$

In the same way,

$$hK_{1,L}W r_{1,L}(0) = \beta_{1,L}u_{1,L}^+(0),$$

with,

$$(5.7) \quad \beta_{1,L} := \frac{1}{h\mathcal{W}(u_{1,L}^+, u_{1,L}^-)} \int_{-\infty}^0 u_{1,L}^-(t)(W r_{1,L})(t)dt.$$

In addition, we can write,

$$r_{1,L}(x) = -\alpha_{1,L}u_{2,L}^+(x) + \tilde{r}_{1,L}(x)$$

with,

$$\begin{aligned} \tilde{r}_{1,L}(x) := & \frac{1}{h\mathcal{W}(u_{2,L}^+, u_{2,L}^-)} \int_0^x \left(u_{2,L}^+(x)u_{2,L}^-(t) - u_{2,L}^-(x)u_{2,L}^+(t) \right) \\ & \times (W^*u_{1,L}^-)(t)dt. \end{aligned}$$

In particular $\tilde{r}_{1,L}'(0) = 0$, and thus $r_{1,L}'(0) = -\alpha_{1,L}(u_{2,L}^+)'(0)$. We see in the same way that $(hK_{1,L}W r_{1,L})'(0) = \beta_{1,L}(u_{1,L}^+)'(0)$.

Moreover, concerning the remainder term in the derivative, we observe that for any j, S , one has $\tilde{\partial}u_{j,S}^\pm(0) = \mathcal{O}(1)$ (see, e.g., Remark 8.3). Therefore, for any $v \in C_b^0(I_L)$, we see from the definitions of M_L and $K_{2,L}$ that we have,

$$\begin{aligned} \tilde{\partial}(hK_{2,L}W^*v)(0) &= \mathcal{O}(\varepsilon^{-1}) \left(\int_{-\infty}^0 |u_{2,L}^-(t)| \cdot |v(t)| dt + h|(u_{2,L}^-)'(0)| \cdot |v(0)| \right); \\ \tilde{\partial}M_L v(0) &= \mathcal{O}(\varepsilon^{-2}) \left(\iint_{-\infty}^0 |U_2(t, s)| \cdot |v(s)| dt ds + h \int_{-\infty}^0 |U_2(t, 0)| \cdot |v(0)| dt \right), \end{aligned}$$

where U_2 is defined in (3.6). Then, we observe that $\int_{-\infty}^0 |u_{2,L}^-(t)| dt = \mathcal{O}(\varepsilon^2)$ and, with the same proof as for (3.15), we have $\iint_{-\infty}^0 |U_2(t, s)| dt ds = \mathcal{O}(\varepsilon^4)$. Using also (3.11), we obtain,

$$\begin{aligned} \tilde{\partial}(hK_{2,L}W^*v)(0) &= \mathcal{O}(\varepsilon) \sup_{I_L} |v|; \\ \tilde{\partial}M_L v(0) &= \mathcal{O}(\varepsilon^2) \sup_{I_L} |v|. \end{aligned}$$

As a consequence,

$$\begin{aligned}\tilde{\partial}(hK_{2,L}W^*\sum_{j\geq 1}M_L^ju_{1,L}^-)(0) &= \mathcal{O}(\varepsilon^3); \\ \tilde{\partial}(\sum_{j\geq 2}M_L^ju_{1,L}^-)(0) &= \mathcal{O}(\varepsilon^4),\end{aligned}$$

and (5.3) follows. The proof of (5.4) is almost the same, with the only difference that the starting function is $hK_{1,L}Wu_{2,L}^-$ instead of $u_{1,L}^-$. But thanks to the decay properties of $u_{2,L}^-$, we see that its behaviour is similar to that of $u_{1,L}^-$, and (5.4) follows.

In addition to (5.6)-(5.7), the other constants appearing in (5.3)-(5.4) are,

$$\begin{aligned}\alpha_{2,L} &= \frac{-\int_{-\infty}^0 u_{1,L}^-(t)(Wu_{2,L}^-)(t)dt}{h\mathcal{W}(u_{1,L}^+, u_{1,L}^-)} \quad ; \quad \beta_{2,L} = \frac{\int_{-\infty}^0 u_{2,L}^-(t)(W^*r_{2,L})(t)dt}{h\mathcal{W}(u_{2,L}^+, u_{2,L}^-)}; \\ \alpha_{1,R} &= \frac{-\int_0^{+\infty} u_{2,R}^-(t)(W^*u_{1,R}^-)(t)dt}{h\mathcal{W}(u_{2,R}^-, u_{2,R}^+)} \quad ; \quad \beta_{1,R} = \frac{\int_0^{+\infty} u_{1,R}^-(t)(Wr_{1,R})(t)dt}{h\mathcal{W}(u_{1,R}^-, u_{1,R}^+)}; \\ \alpha_{2,R} &= \frac{-\int_0^{+\infty} u_{1,R}^-(t)(Wu_{2,R}^-)(t)dt}{h\mathcal{W}(u_{1,R}^-, u_{1,R}^+)} \quad ; \quad \beta_{2,R} = \frac{\int_0^{+\infty} u_{2,R}^-(t)(W^*r_{2,R})(t)dt}{h\mathcal{W}(u_{2,R}^-, u_{2,R}^+)} ,\end{aligned}$$

where we have set,

$$r_{2,L} := hK_{1,L}Wu_{2,L}^- \quad ; \quad r_{1,R} := hK_{2,R}W^*u_{1,R}^- \quad ; \quad r_{2,R} := hK_{1,R}Wu_{2,R}^- ,$$

and where, in the case of $\alpha_{j,R}$ and $\beta_{j,R}$, the integrals run over I_R^θ . \square

Now, setting,

$$\begin{aligned}\mu_A(t) &:= \int_0^{+\infty} \text{Ai}(y-t)\check{\text{Ai}}(y+t)dy; \\ \mu_B(t) &:= \int_0^{+\infty} \text{Ai}(y-t)\check{\text{Bi}}(y+t)dy,\end{aligned}\tag{5.9}$$

we also have,

Proposition 5.3. *As $h \rightarrow 0_+$, one has,*

(5.10)

$$\begin{aligned}\alpha_{j,L} &= -2\varepsilon\pi r_0(0) \left(\mu_A(\text{Re } \rho) \sin \frac{\mathcal{A}(E)}{h} + \mu_B(\text{Re } \rho) \cos \frac{\mathcal{A}(E)}{h} \right) + \mathcal{O}(\varepsilon^2), \\ \alpha_{j,R} &= -\frac{\varepsilon\pi r_0(0)e^{i\frac{\pi}{4}}}{\sqrt{2}} (\mu_A(\text{Re } \rho) - i\mu_B(\text{Re } \rho)) + \mathcal{O}(\varepsilon^2), \quad (j = 1, 2); \\ \text{Im } \beta_{1,L} &= \mathcal{O}(h); \\ \text{Im } \beta_{1,R} &= \pi^2 r_0(0)^2 \varepsilon^2 (\mu_A(\text{Re } \rho)^2 + \mu_B(\text{Re } \rho)^2) + \mathcal{O}(h) \\ \text{Re } \beta_{1,R} &= 2\varepsilon^2 \pi^2 r_0(0)^2 \int \int_{0 \leq s \leq t} \text{Ai}(t - \text{Re } \rho) \text{Ai}(s - \text{Re } \rho) \\ &\quad \times (\check{\text{Ai}}(t + \text{Re } \rho) \check{\text{Bi}}(s + \text{Re } \rho) - \check{\text{Ai}}(s + \text{Re } \rho) \check{\text{Bi}}(t + \text{Re } \rho)) ds dt + \mathcal{O}(h); \\ \beta_{2,S} &= \mathcal{O}(\varepsilon^2), \quad (S = L, R).\end{aligned}$$

Proof. Let us first study $\alpha_{1,L}$ given in (5.6). Using (3.2) and the exponential decay of $u_{2,L}^-$ away from 0, we obtain,

$$\alpha_{1,L} = \frac{-\pi}{2\varepsilon} \int_{-\delta}^0 u_{2,L}^-(t) (r_0(t) u_{1,L}^-(t) + h D_t(\bar{r}_1 u_{1,L}^-(t))) dt + \mathcal{O}(\varepsilon^2),$$

where $\delta > 0$ is arbitrarily small. Further, an integration by parts gives,

$$\alpha_{1,L} = \frac{-\pi}{2\varepsilon} \int_{-\delta}^0 u_{2,L}^-(t) r_0(t) u_{1,L}^-(t) + i h (u_{2,L}^-)'(t) \bar{r}_1(t) u_{1,L}^-(t) dt + \mathcal{O}(\varepsilon^2),$$

and since $h(u_{2,L}^-)'(t) u_{1,L}^-(t)$ is $\mathcal{O}(h^{1/3} e^{-c|t|^{3/2}/h})$ on $[-\delta, -Ch^{2/3}]$ (with $c > 0$, and $C > 1$ large enough), and is $\mathcal{O}(h^{1/3})$ on $[-Ch^{2/3}, 0]$, we are reduced to,

$$(5.11) \quad \alpha_{1,L} = \frac{-\pi}{2\varepsilon} \int_{-\delta}^0 u_{2,L}^-(t) r_0(t) u_{1,L}^-(t) dt + \mathcal{O}(\varepsilon^2).$$

We introduce a large extra-parameter $\lambda \gg 1$, and, dividing the integral in two parts, we set,

$$\begin{aligned} \alpha_{1,L}^-(\lambda) &= \frac{-\pi}{2\varepsilon} \int_{-\delta}^{-\lambda h^{\frac{2}{3}}} u_{2,L}^-(t) r_0(t) u_{1,L}^-(t) dt; \\ \alpha_{1,L}^+(\lambda) &= \frac{-\pi}{2\varepsilon} \int_{-\lambda h^{\frac{2}{3}}}^0 u_{2,L}^-(t) r_0(t) u_{1,L}^-(t) dt. \end{aligned}$$

We have,

$$\alpha_{1,L}^-(\lambda) = \mathcal{O}(\varepsilon^{-1}) \int_{\lambda h^{\frac{2}{3}}}^{\delta} \frac{h^{\frac{1}{3}}}{\sqrt{t}} e^{-ct^{3/2}/h} dt = \mathcal{O}(\varepsilon e^{-c\lambda^{3/2}}),$$

where $c > 0$ is a constant, and the estimate is uniform with respect to $\varepsilon > 0$ small enough and $\lambda > 1$ large enough such that $\lambda h^{2/3} \rightarrow 0$. In particular, taking,

$$(5.12) \quad \lambda \geq (c^{-1} |\ln \varepsilon|)^{2/3},$$

we obtain,

$$\alpha_{1,L}^-(\lambda) = \mathcal{O}(\varepsilon^2).$$

On the other hand, using Propositions 5.1, 8.2 and 8.5, we obtain,

$$\begin{aligned} \alpha_{1,L}^+(\lambda) &= \frac{-2\pi}{\varepsilon} \left(\sin \frac{\mathcal{A}}{h} \right) \int_{-\lambda h^{\frac{2}{3}}}^0 r_0(t) (\xi_1' \xi_2')^{-\frac{1}{2}} \text{Ai}(h^{-\frac{2}{3}} \xi_1) \check{\text{Ai}}(h^{-\frac{2}{3}} \xi_2) dt \\ &\quad - \frac{2\pi}{\varepsilon} \left(\cos \frac{\mathcal{A}}{h} \right) \int_{-\lambda h^{\frac{2}{3}}}^0 r_0(t) (\xi_1' \xi_2')^{-\frac{1}{2}} \text{Bi}(h^{-\frac{2}{3}} \xi_1) \check{\text{Ai}}(h^{-\frac{2}{3}} \xi_2) dt + \mathcal{O}(\varepsilon^2). \end{aligned}$$

Making the change of variable $y := \varepsilon^{-2} t$, and using that, for $y \in [-\lambda, 0]$, we have $r_0(\varepsilon^2 y) = r_0(0) + \mathcal{O}(\varepsilon^2 \lambda)$, $\xi_j'(\varepsilon^2 y) = 1 + \mathcal{O}(\varepsilon^2 \lambda)$, $\text{Ai}(\varepsilon^{-2} \xi_1(\varepsilon^2 y)) = \text{Ai}(y - \rho) + \mathcal{O}(\lambda^2 \varepsilon^2)$, $\check{\text{Ai}}(\varepsilon^{-2} \xi_2(\varepsilon^2 y)) = \check{\text{Ai}}(y + \rho) + \mathcal{O}(\lambda^2 \varepsilon^2)$, $\text{Bi}(\varepsilon^{-2} \xi_1(\varepsilon^2 y)) = \text{Bi}(y - \rho) + \mathcal{O}(\lambda^2 \varepsilon^2)$, we obtain,

$$\begin{aligned} \alpha_{1,L}^+(\lambda) &= -2\varepsilon \pi r_0(0) \left(\sin \frac{\mathcal{A}}{h} \right) \int_{-\lambda}^0 \text{Ai}(y - \rho) \check{\text{Ai}}(y + \rho) dy \\ &\quad - 2\varepsilon \pi r_0(0) \left(\cos \frac{\mathcal{A}}{h} \right) \int_{-\lambda}^0 \text{Bi}(y - \rho) \check{\text{Ai}}(y + \rho) dy + \mathcal{O}(\varepsilon^2) + \mathcal{O}(\lambda^3 \varepsilon^3). \end{aligned}$$

Then, using the behaviour of Ai , $\check{\text{Ai}}$ and Bi at $-\infty$, this leads to,

$$\begin{aligned} \alpha_{1,L}^+(\lambda) &= -2\varepsilon\pi r_0(0) \int_{-\infty}^0 \check{\text{Ai}}(y+\rho) \left(\left(\sin \frac{\mathcal{A}}{h}\right) \text{Ai}(y-\rho) + \left(\cos \frac{\mathcal{A}}{h}\right) \text{Bi}(y-\rho) \right) dy \\ &\quad + \mathcal{O}(\varepsilon e^{-c'\lambda^{3/2}}) + \mathcal{O}(\varepsilon^2) + \mathcal{O}(\lambda^3 \varepsilon^3), \end{aligned}$$

with $c' > 0$ constant. Therefore, taking $\lambda := ((c'')^{-1} |\ln \varepsilon|)^{2/3}$ with $c'' = \min\{c, c'\}$, and using the fact that $\text{Im } \rho = \mathcal{O}(\varepsilon)$, we obtain the required approximation of $\alpha_{1,L}$. The approximations of $\alpha_{2,L}$, $\alpha_{1,R}$ and $\alpha_{2,R}$ are obtained in a very similar way (starting from (5.8)), and we omit the proofs.

Now we study $\beta_{1,R}$. We have,

$$\begin{aligned} \beta_{1,R} &= \frac{\pi^2}{4\varepsilon^2} \int_0^{+\infty} u_{1,R}^-(t) W(t, hD_t) \left[u_{2,R}^-(t) \int_0^t u_{2,R}^+(s) (W^* u_{1,R}^-)(s) ds \right. \\ &\quad \left. + u_{2,R}^+(t) (W^* u_{1,R}^-)(s) ds \int_t^{+\infty} u_{2,R}^-(s) (W^* u_{1,R}^-)(s) ds \right] dt + \mathcal{O}(h), \end{aligned}$$

where the integrals run over I_R^θ . Because of the exponential decay of $u_{1,R}^-$ away from 0, we immediately see that only a neighbourhood of 0 contributes to the integrals (up to $\mathcal{O}(e^{-c/h})$ with $c > 0$). Moreover, making an integration by parts and using the behaviour of all the functions near 0, we see as for $\alpha_{1,L}$ that, up to an error $\mathcal{O}(\varepsilon^3)$, W and W^* can be replaced by r_0 . Finally, using (3.16) and the expressions of $u_{1,R}^-$, $u_{2,L}^-$ and $u_{2,L}^+$ given in Propositions 8.2 and 8.5, and proceeding as for $\alpha_{1,L}$, we obtain,

$$\begin{aligned} \beta_{1,R} &= 2i\pi^2 r_0(0)^2 \varepsilon^2 \iint_{0 \leq s \leq t} \text{Ai}(t-\rho) \text{Ai}(s-\rho) \check{\text{A}}_{out}(t+\rho) \check{\text{A}}_{in}(s+\rho) ds dt \\ &\quad + 2i\pi^2 r_0(0)^2 \varepsilon^2 \iint_{0 \leq t \leq s} \text{Ai}(t-\rho) \text{Ai}(s-\rho) \check{\text{A}}_{in}(t+\rho) \check{\text{A}}_{out}(s+\rho) ds dt \\ &\quad + \mathcal{O}(h), \end{aligned}$$

where we have set,

$$\check{\text{A}}_{out} := \check{\text{Ai}} - i\check{\text{Bi}} \quad ; \quad \check{\text{A}}_{in} := \check{\text{Ai}} + i\check{\text{Bi}}.$$

Exchanging t and s in the second integral, and replacing $\check{\text{A}}_{out}$ and $\check{\text{A}}_{in}$ by their expressions, an elementary computation (plus the fact that $\text{Im } \rho = \mathcal{O}(\varepsilon)$) leads to the required approximation of $\beta_{1,R}$.

The same procedure (but somehow simpler) shows that $\beta_{1,L}$, $\beta_{2,L}$ and $\beta_{2,R}$ are $\mathcal{O}(\varepsilon^2)$ (note that, for $\beta_{1,L}$ and $\beta_{2,R}$, one must use the fact that the integral $\int_0^\infty \int_0^\infty (ts)^{-\frac{1}{2}} e^{-|t^{\frac{3}{2}} - s^{\frac{3}{2}}|} dt ds$ is finite). Finally, concerning $\beta_{1,L}$, we see on (5.7) that it only involves functions $u_{j,L}^\pm$ that are real when E is real, and since by assumption r_0 is real on the real, the same kind of estimates as for $\beta_{1,R}$ show that it is real up to $\mathcal{O}(h)$. \square

6. QUANTIZATION CONDITION

In order to simplify the writing, we will use the following notation:

If u_1 is any of the functions $u_{1,L}^\pm$ or $u_{1,R}^\pm$, we set,

$$\mathbf{u}_1 := \begin{bmatrix} u_1(0) \\ \tilde{\partial}u_1(0) \\ 0 \\ 0 \end{bmatrix},$$

and if u_2 is any of the functions $u_{2,L}^\pm$ or $u_{2,R}^\pm$, we set,

$$\mathbf{u}_2 := \begin{bmatrix} 0 \\ 0 \\ u_2(0) \\ \tilde{\partial}u_2(0) \end{bmatrix}.$$

With this notation, we see on Proposition 5.2 that we have,

(6.1)

$$\mathcal{W}_0(E) := \widetilde{\mathcal{W}}(w_{1,L}, w_{2,L}, w_{1,R}, w_{2,R}) = \det(\mathbf{v}_{1,L}, \mathbf{v}_{1,R}, \mathbf{v}_{2,L}, \mathbf{v}_{2,R}) + \mathcal{O}(h),$$

with,

$$\mathbf{v}_{1,S} := \mathbf{u}_{1,S}^- + \alpha_{1,S}\mathbf{u}_{2,S}^+ + \beta_{1,S}\mathbf{u}_{1,S}^+;$$

$$\mathbf{v}_{2,S} := \mathbf{u}_{2,S}^- + \alpha_{2,S}\mathbf{u}_{1,S}^+ + \beta_{2,S}\mathbf{u}_{2,S}^+ \quad (S = L, R).$$

Developing the determinant by multi-linearity, and observing that all the terms that involve at least three vectors with the same value of the index j vanish, we obtain,

$$\begin{aligned} \mathcal{W}_0(E) = & \widetilde{\mathcal{W}}(u_{1,L}^-, u_{1,R}^-) \widetilde{\mathcal{W}}(u_{2,L}^-, u_{2,R}^-) \\ & + \beta_{2,R} \widetilde{\mathcal{W}}(u_{1,L}^-, u_{1,R}^-) \widetilde{\mathcal{W}}(u_{2,L}^-, u_{2,R}^+) \\ & + \beta_{2,L} \widetilde{\mathcal{W}}(u_{1,L}^-, u_{1,R}^-) \widetilde{\mathcal{W}}(u_{2,L}^+, u_{2,R}^-) \\ & + \alpha_{1,R} \alpha_{2,R} \widetilde{\mathcal{W}}(u_{1,L}^-, u_{1,R}^+) \widetilde{\mathcal{W}}(u_{2,R}^+, u_{2,L}^-) \\ & + \alpha_{1,R} \alpha_{2,L} \widetilde{\mathcal{W}}(u_{1,L}^-, u_{1,R}^+) \widetilde{\mathcal{W}}(u_{2,R}^-, u_{2,L}^+) \\ & + \beta_{1,R} \widetilde{\mathcal{W}}(u_{1,L}^-, u_{1,R}^+) \widetilde{\mathcal{W}}(u_{2,L}^-, u_{2,R}^-) \\ & + \alpha_{1,L} \alpha_{2,R} \widetilde{\mathcal{W}}(u_{2,L}^+, u_{2,R}^-) \widetilde{\mathcal{W}}(u_{1,R}^+, u_{1,L}^-) \\ & + \alpha_{1,L} \alpha_{2,L} \widetilde{\mathcal{W}}(u_{2,L}^+, u_{2,R}^-) \widetilde{\mathcal{W}}(u_{1,R}^-, u_{1,L}^+) \\ & + \beta_{1,L} \widetilde{\mathcal{W}}(u_{1,L}^+, u_{1,R}^-) \widetilde{\mathcal{W}}(u_{2,L}^-, u_{2,R}^-) + \mathcal{O}(h). \end{aligned}$$

In particular, we observe that each $\alpha_{j,S}$ is always multiplied by another similar quantity, that is, by $\mathcal{O}(\varepsilon)$. As a consequence, an error on $\alpha_{j,S}$ of order ε^2 will lead to an error of order h in $\mathcal{W}_0(E)$, and thus, by Proposition 5.3, we can replace $\alpha_{2,S}$ by $\alpha_{1,S}$ ($S = L, R$). Then, computing the various Wronskians that appear (see Appendix 8.3), we find,

(6.2)

$$\begin{aligned} -i\pi^2 e^{-i\frac{\pi}{4}} \mathcal{W}_0(E) = & -4\sqrt{2}(\cos \frac{\mathcal{A}}{h})(1 + \mathcal{O}(\varepsilon^2)) + 4\sqrt{2}(\sin \frac{\mathcal{A}}{h})\alpha_{1,R}^2 \\ & + 8e^{\frac{i\pi}{4}}\alpha_{1,R}\alpha_{1,L} + 2\sqrt{2}(\sin \frac{\mathcal{A}}{h})\beta_{1,R} + i\sqrt{2}(\sin \frac{\mathcal{A}}{h})\alpha_{1,L}^2 \\ & + 2\sqrt{2}(\sin \frac{\mathcal{A}}{h})\beta_{1,L} + \mathcal{O}(h). \end{aligned}$$

Finally, observing that we have,

$$\begin{aligned}\alpha_{1,R}^2 &= \frac{\pi^2 r_0(0)^2 \varepsilon^2}{2} (2\mu_A \mu_B + i\mu_A^2 - i\mu_B^2) + \mathcal{O}(h); \\ \alpha_{1,L} \alpha_{1,R} &= \pi^2 r_0(0)^2 \varepsilon^2 \sqrt{2} e^{i\frac{\pi}{4}} \left(\sin \frac{\mathcal{A}}{h} \right) \mu_A (\mu_A - i\mu_B) + \mathcal{O}(h + \varepsilon^2 |\cos \frac{\mathcal{A}}{h}|); \\ \alpha_{1,L}^2 &= 4\pi^2 r_0(0)^2 \varepsilon^2 \left(\sin \frac{\mathcal{A}}{h} \right)^2 \mu_A^2 + \mathcal{O}(h + \varepsilon^2 |\cos \frac{\mathcal{A}}{h}|); \\ \beta_{1,R} &= \operatorname{Re} \beta_{1,R} + i\pi^2 r_0(0)^2 \varepsilon^2 (\mu_A^2 + \mu_B^2) + \mathcal{O}(h); \\ \beta_{1,L} &= \operatorname{Re} \beta_{1,L} + \mathcal{O}(h),\end{aligned}$$

we obtain,

$$\begin{aligned}(6.3) \quad -i\pi^2 e^{-i\frac{\pi}{4}} \mathcal{W}_0(E) &= -4\sqrt{2} \left(\cos \frac{\mathcal{A}}{h} \right) (1 + \mathcal{O}(\varepsilon^2)) + 2\sqrt{2} \left(\sin \frac{\mathcal{A}}{h} \right) \operatorname{Re} (\beta_{1,L} + \beta_{1,R}) \\ &\quad + 4\sqrt{2} (\pi r_0(0) \varepsilon)^2 \left(\sin \frac{\mathcal{A}}{h} \right) \left(3\mu_A \mu_B + i(3 + \sin^2 \frac{\mathcal{A}}{h}) \mu_A^2 \right) \\ &\quad + \mathcal{O}(h).\end{aligned}$$

Now, by Proposition 4.2, the quantization condition reads,

$$\mathcal{W}_0(E) = 0.$$

Hence, in view of (6.2) and of Proposition 5.2, if we set,

$$b_0 := \frac{1}{2\varepsilon^2} \operatorname{Re}(\beta_{1,L} + \beta_{1,R}) + 3\pi^2 r_0(0)^2 \mu_A (\operatorname{Re} \rho) \mu_B (\operatorname{Re} \rho) = \mathcal{O}(1),$$

we have proved,

Proposition 6.1. *$E = \rho\varepsilon^2 \in \mathcal{D}_h(C_0)$ is a resonance of P if and only if,*

$$(6.4) \quad \cos \frac{\mathcal{A}(E)}{\varepsilon^3} = \varepsilon^2 F(E, \varepsilon),$$

where

$$(6.5) \quad F(E, \varepsilon) = \left(b_0 + i\pi^2 r_0(0)^2 (3 + \sin^2 \frac{\mathcal{A}(E)}{\varepsilon^3}) \mu_A (\operatorname{Re} \rho)^2 \right) \sin \frac{\mathcal{A}(E)}{\varepsilon^3} + \mathcal{O}(\varepsilon).$$

Remark 6.1. *The quantization condition (6.4) is of Bohr-Sommerfeld type associated with the single potential well of $V_1(x)$. The imaginary part of $F(E, \varepsilon)$ will give an estimate on the width of resonances.*

7. COMPLETION OF THE PROOF

In order to solve (6.4) in $\mathcal{D}_h(C_0)$ (where C_0 may actually vary a little bit in order to avoid "border" effects), we first observe that, near $E = 0$, the roots of the equation $\cos(\mathcal{A}(E)/h) = 0$ are given by $E = e_k(h)$ with,

$$e_k(h) := \mathcal{A}^{-1} \left(\left(k + \frac{1}{2} \right) \pi h \right) \in \mathbb{R} \quad (k \in \mathbb{Z}).$$

(Here, $k \in \mathbb{Z}$ must be taken such a way that $\mathcal{A}^{-1}((k + \frac{1}{2})\pi h)$ is effectively close to 0.) In particular, restricting to $E = \mathcal{O}(\varepsilon^2)$, and writing $\mathcal{A}(E) = \mathcal{A}(0) + E\mathcal{A}'(0) + \frac{1}{2}E^2\mathcal{A}''(0) + \mathcal{O}(E^3)$, we obtain the well known relation,

$$e_k(h) = \lambda_k(h)\varepsilon^2 - \frac{\lambda_k(h)^2\mathcal{A}''(0)}{2\mathcal{A}'(0)}\varepsilon^4 + \mathcal{O}(\varepsilon^6),$$

where $\lambda_k(h)$ is defined in (2.3). In particular, the distance between two consecutive $e_k(h)$'s is of order h . Moreover, if $E \in \mathbb{C}$ is such that $E = \mathcal{O}(\varepsilon^2)$ and $\mathcal{A}(E)$ stays at a distance greater than δh from the set $\{e_k(h); k \in \mathbb{Z}\}$, with $\delta > 0$ constant, then $\cos(\mathcal{A}(E)/h)$ remains at some fix positive distance from 0. As a consequence, for $\varepsilon > 0$ small enough, we can apply the Rouché theorem and conclude that, for each k such that $\lambda_k(h) = \mathcal{O}(1)$, there exists a unique solution $E_k(h)$ to (6.4) such that,

$$E_k(h) = e_k(h) + o(h),$$

and, conversely, all the roots of (6.4) in $\mathcal{D}_h(C_0)$ are of this type.

Now, going back to equation (6.4), we immediately see that, actually, we have,

$$E_k(h) = e_k(h) + \mathcal{O}(\varepsilon^5),$$

so that (2.4) is proved in the case $\tau_1 = \tau_2 = 1$

In order to prove (2.5), we first observe that, by (2.4), the equation (6.4) implies,

$$\cos \frac{\mathcal{A}(E_k(h))}{\varepsilon^3} = \varepsilon^2 F(\lambda_k(h)\varepsilon^2, \varepsilon) + \mathcal{O}(\varepsilon^3).$$

Then, taking the local inverse of \cos near $(k + \frac{1}{2})\pi$, and the inverse of \mathcal{A} near $E = 0$, (2.5) (with $\tau_1 = \tau_2 = 1$) immediately follows from (6.5) and the fact that $\sin \frac{\mathcal{A}(\lambda_k(h)\varepsilon^2)}{\varepsilon^3} = (-1)^k + \mathcal{O}(\varepsilon^2)$.

When τ_1 and τ_2 are general positive numbers, we observe that all the constructions Sections 3.1 to 5 and of Appendix 8.2 remain completely unchanged. Therefore, the proof proceeds exactly in the same way, and the only differences are in the approximate values of $\xi_1(\varepsilon^{-2}y)$ and $\xi_2(\varepsilon^{-2}y)$. A very simple computation shows that they become,

$$\begin{aligned} \xi_1(\varepsilon^{-2}y) &= \tau_1^{\frac{1}{3}} \left(y - \frac{\rho}{\tau_1} \right) + \mathcal{O}(\varepsilon^2); \\ \xi_2(\varepsilon^{-2}y) &= \tau_2^{\frac{1}{3}} \left(y + \frac{\rho}{\tau_2} \right) + \mathcal{O}(\varepsilon^2). \end{aligned}$$

As a consequence, the approximations given in (5.10) have to be changed, too, and indeed now the functions μ_A and μ_B will depend also on the side where we are working (on I_L or on I_R). On I_R (that is, for $\alpha_{1,R}$ and $\beta_{1,R}$) they will just be as before, with $\text{Ai}(y - \rho)$, $\text{Bi}(y - \rho)$ substituted by $\text{Ai}(\tau_1^{-2/3}(\tau_1 y - \rho))$, $\text{Bi}(\tau_1^{-2/3}(\tau_1 y - \rho))$, and $\check{\text{Ai}}(y + \rho)$, $\check{\text{Bi}}(y + \rho)$ substituted by $\check{\text{Ai}}(\tau_2^{-2/3}(\tau_2 y + \rho))$, $\check{\text{Bi}}(\tau_2^{-2/3}(\tau_2 y + \rho))$. On I_L (that is, for $\alpha_{1,L}$), μ_A and

μ_B become,

$$\begin{aligned}\tilde{\mu}_A(t) &= \int_{-\infty}^0 \text{Ai}(\tau_1^{-2/3}(\tau_1 y - \rho)) \check{\text{Ai}}(\tau_2^{-2/3}(\tau_2 y + \rho)) dy; \\ \tilde{\mu}_B(t) &= \int_{-\infty}^0 \text{Bi}(\tau_1^{-2/3}(\tau_1 y - \rho)) \check{\text{Ai}}(\tau_2^{-2/3}(\tau_2 y + \rho)) dy.\end{aligned}$$

But the computations proceed in a similar way, and since $\tilde{\mu}_A(t) = \mu_2(t)$, the result follows in the general case, too.

Remark 7.1. Resonant states *By construction, the resonant state φ_k associated with $E_k(h)$ can be written both as a linear combination of $w_{1,L}$ and $w_{2,L}$, and a linear combination of $w_{1,R}$ and $w_{2,R}$ (all computed at $E = E_k(h)$). The coefficients can actually be computed (up to $\mathcal{O}(h)$) by using Proposition 5.3, identifying each $w_{j,S}$ with the vector $\vec{w}_{j,L}$ of \mathbb{R}^4 given by,*

$$\vec{w}_{j,L} := \begin{bmatrix} w_{j,S}^-(0) \\ \tilde{\partial} w_{j,S}^-(0) \end{bmatrix}.$$

Then, the approximations of the various functions involved with their Airy representation (obtained from Propositions 8.2 and 8.5) permit us to write φ_k as,

$$(7.1) \quad \varphi_k = w_{1,L} - \mu w_{2,L} = \lambda w_{1,R} + \nu w_{2,R},$$

with,

$$\begin{aligned}\lambda &= \sin \frac{\mathcal{A}}{h} + \mathcal{O}(h) = (-1)^k + \mathcal{O}(\varepsilon^2); \\ \nu &= -2\lambda\alpha_{1,R} + \mathcal{O}(h) = 4\varepsilon\pi r_0(0)\mu_A(\lambda_k(h)) + \mathcal{O}(h); \\ \mu &= \cos \frac{\mathcal{A}}{h} - \frac{1}{2}(\beta_{1,L} + \lambda\beta_{1,R} + \nu\alpha_{2,R}) + \mathcal{O}(h) = \mathcal{O}(\varepsilon^2).\end{aligned}$$

Using the various asymptotic behaviours of the functions $w_{j,S}$'s, one can derive the (semiclassical) asymptotic behaviour of φ_k in all of \mathbb{R} .

8. APPENDIX

8.1. Inhomogeneous Airy equations. Let $\text{Ai}(y)$ be the Airy function, which is characterised as the solution to the Airy equation

$$(8.1) \quad -u''(y) + yu(y) = 0$$

with exponential decay as y tends to $+\infty$,

$$\text{Ai}(y) = \frac{1}{2\sqrt{\pi}} y^{-\frac{1}{4}} e^{-\frac{2}{3}y^{3/2}} (1 + \mathcal{O}(y^{-1})) \quad (y \rightarrow +\infty).$$

It is oscillating when $y < 0$, and its behaviour is,

$$\text{Ai}(y) = \frac{1}{\sqrt{\pi}} (-y)^{-\frac{1}{4}} \sin \left(\frac{2}{3}(-y)^{3/2} + \frac{\pi}{4} \right) (1 + \mathcal{O}(|y|^{-1})) \quad \text{as } y \rightarrow -\infty.$$

Moreover, the asymptotic behaviour of its derivative $\text{Ai}'(y)$ is obtained by formally differentiating the previous ones, and these asymptotic behaviours remain valid in sufficiently small complex sectors around the real line.

We define another solution $\text{Bi}(y)$ to the Airy equation by the asymptotic behavior as $y \rightarrow -\infty$

$$\text{Bi}(y) = \frac{-1}{\sqrt{\pi}} (-y)^{-\frac{1}{4}} \sin\left(\frac{2}{3}(-y)^{3/2} - \frac{\pi}{4}\right) (1 + \mathcal{O}(|y|^{-1})) \quad (y \rightarrow -\infty).$$

$\text{Bi}(y)$ is positive and grows exponentially for $y > 0$, and satisfies

$$\text{Bi}(y) = \frac{1}{\sqrt{\pi}} y^{-\frac{1}{4}} e^{\frac{2}{3}y^{3/2}} (1 + \mathcal{O}(y^{-1})) \quad (y \rightarrow +\infty).$$

From the asymptotic behaviors of $\text{Ai}(y)$ and $\text{Bi}(y)$ as $y \rightarrow -\infty$, we easily see the following properties. At first, the solutions

$$(8.2) \quad \text{Ai}(y) - i\text{Bi}(y) \sim \frac{e^{-\pi i/4}}{\sqrt{\pi}} (-y)^{-\frac{1}{4}} \exp\left(\frac{2i}{3}(-y)^{3/2}\right) \quad (y \rightarrow -\infty);$$

$$(8.3) \quad \text{Ai}(y) + i\text{Bi}(y) \sim \frac{e^{\pi i/4}}{\sqrt{\pi}} (-y)^{-\frac{1}{4}} \exp\left(-\frac{2i}{3}(-y)^{3/2}\right) \quad (y \rightarrow -\infty),$$

are outgoing and incoming respectively for negative y , and secondly, the wronskian of $\text{Ai}(y)$ and $\text{Bi}(y)$ is given by

$$\mathcal{W}[\text{Ai}, \text{Bi}] := \text{Ai}(y)\text{Bi}'(y) - \text{Ai}'(y)\text{Bi}(y) = \pi^{-1}.$$

Set

$$K(y, z) := -\pi \{ \text{Ai}(y)\text{Bi}(z) - \text{Ai}(z)\text{Bi}(y) \},$$

and define the integral operators \mathcal{K} and $\tilde{\mathcal{K}}$ for $f \in C_0^\infty(\mathbb{R})$

$$(8.4) \quad \mathcal{K}[f](y) := \int_y^0 K(y, z)f(z)dz; \quad \tilde{\mathcal{K}}[f](y) := \int_0^y K(-y, -z)f(z)dz.$$

The function $\mathcal{K}[f](y)$ gives a particular solution to the inhomogeneous equation

$$-u'' + yu = f,$$

while $\tilde{\mathcal{K}}[f](y)$ gives a particular solution to

$$-u'' - yu = f.$$

Notice that there exists a symmetric property between \mathcal{K} and $\tilde{\mathcal{K}}$, namely,

$$(8.5) \quad \mathcal{K}[f](-y) = \tilde{\mathcal{K}}[\check{f}](y),$$

where $\check{f}(y) = f(-y)$. Moreover, if $\rho \in \mathbb{C}$, then the operators \mathcal{K}_ρ and $\tilde{\mathcal{K}}_\rho$ defined by,

$$(8.6) \quad \mathcal{K}_\rho[f](y) := \int_y^0 K(y-\rho, z-\rho)f(z)dz; \quad \tilde{\mathcal{K}}_\rho[f](y) := \int_0^y K(-y-\rho, -z-\rho)f(z)dz$$

give solutions to the equations

$$-u'' + (y-\rho)u = f \quad ; \quad -u'' - (y+\rho)u = f,$$

respectively.

Remark 8.1. Observe that all these constructions remain valid when y becomes complex, as long as $\text{Im } y$ stays bounded. In that case, the integrals must be taken along any complex curve joining y to 0.

8.2. Yafaev's constructions. In this appendix, we recall and extend the constructions made in [24] for the scalar Schrödinger equation $(P_j - E)u = 0$. In [24] such constructions are made for real E only, and they just concern solutions decaying at infinity. Here, we need to consider complex values of E and exponentially large or oscillating solutions, too.

We fix $x_0 \in (x^*, 0)$, and we first treat the case $j = 1$. For E small enough, we denote by $x_1 = x_1(E)$ the only point near 0 where $V_1 - E$ vanishes (in particular, $x_1(E) = E + \mathcal{O}(E^2)$ depends analytically on E). In the particular case where E is real, we can define as in [24],

$$(8.7) \quad \begin{aligned} \xi_1(x; E) &= \left(\frac{3}{2} \int_{x_1(E)}^x \sqrt{V_1(t) - E} dt \right)^{\frac{2}{3}} \quad \text{when } x \geq x_1; \\ \xi_1(x; E) &= - \left(\frac{3}{2} \int_x^{x_1(E)} \sqrt{E - V_1(t)} dt \right)^{\frac{2}{3}} \quad \text{when } x_0 \leq x \leq x_1. \end{aligned}$$

Then, it is easy to check that $\xi_1(x; E) = x - x_1(E) + \mathcal{O}((x - x_1)^2)$ as $x \rightarrow x_1$, and that ξ_1 depends analytically on x and E for $x \in (x_0, +\infty)$, E small enough. Since also V_1 has a positive limit at $+\infty$, we see that we can extend analytically ξ_1 to a complex neighbourhood of $(x_0, +\infty) \times \{0\}$. Then, $\xi_1(x)$ satisfies $(\xi_1')^2 \xi_1 = V_1 - E$ and $\text{Re } \xi_1' > 0$ everywhere on $[x_0, +\infty)$. In particular, when $E \in \mathcal{D}_h(C_0)$ is fixed and x varies in $(x_0, +\infty)$, then ξ_1 describes a smooth complex curve parametrised by x , with $\text{Im } \xi_1(x) = \mathcal{O}(h)$ uniformly. From now on, in order to simplify the notation, we drop the dependence of ξ_1 with respect to E . The result is (see also [24], Theorem 2.5),

Proposition 8.2. *Let $E \in \mathcal{D}_h(C_0)$. Then, the equation $(P_1 - E)u = 0$ admits two real-valued solutions $u_{1,R}^\pm$ on \mathbb{R} , such that, as $x \rightarrow +\infty$, (and uniformly with respect to $h > 0$ small enough),*

$$u_{1,R}^\pm(x) \sim (1 + \mathcal{O}(h)) \frac{h^{\frac{1}{6}}}{\sqrt{\pi}} (V_1(x) - E)^{-1/4} e^{\pm \int_{x_1(E)}^x \sqrt{V_1(t) - E} dt / h},$$

and, as $h \rightarrow 0_+$,

$$\begin{aligned} u_{1,R}^-(x) &= 2(\xi_1'(x))^{-\frac{1}{2}} \text{Ai}(h^{-\frac{2}{3}} \xi_1(x)) (1 + \mathcal{O}(h)) \\ &\quad \text{on } [x_0, +\infty) \cap \{\text{Re } \xi_1(x) \geq 0\}; \\ u_{1,R}^-(x) &= 2(\xi_1'(x))^{-\frac{1}{2}} \text{Ai}(h^{-\frac{2}{3}} \xi_1(x)) + \mathcal{O}(h(1 + h^{-2/3} |\xi_1(x)|)^{-\frac{1}{4}}) \\ &\quad \text{on } [x_0, +\infty) \cap \{\text{Re } \xi_1(x) \leq 0\}; \\ u_{1,R}^+(x) &= (\xi_1'(x))^{-\frac{1}{2}} \text{Bi}(h^{-\frac{2}{3}} \xi_1(x)) (1 + \mathcal{O}(h)) \\ &\quad \text{on } [x_0, +\infty) \cap \{\text{Re } \xi_1(x) \geq 0\}; \\ u_{1,R}^+(x) &= (\xi_1'(x))^{-\frac{1}{2}} \text{Bi}(h^{-\frac{2}{3}} \xi_1(x)) + \mathcal{O}(h(1 + h^{-2/3} |\xi_1(x)|)^{-\frac{1}{4}}) \\ &\quad \text{on } [x_0, +\infty) \cap \{\text{Re } \xi_1(x) \leq 0\}. \end{aligned}$$

Proof. The proof for $u_{1,R}^-$ is the same as in [24], with the difference that, here, E may be complex. However, since we have $\text{Im } E = \mathcal{O}(h)$, all the estimates

in [24] remain valid. Observe, in particular, that when $\operatorname{Re} \xi_1(x) \geq 0$, then $\operatorname{Im}(\xi_1(x))^{3/2} = \mathcal{O}(h)$, and thus $\operatorname{Ai}(h^{-2/3}\xi_1(x)) \neq 0$.

Therefore, let us focus on the construction of $u_{1,R}^+$. As in [24], Section 3, setting $t := h^{-2/3}\xi_1(x)$ and $f(t) := \xi_1'(x)^{1/2}u(x)$, the equation $(P_1 - E)u = 0$ becomes,

$$(8.8) \quad -f''(t) + tf(t) = R(t)f(t),$$

with,

$$(8.9) \quad \begin{aligned} R(t) &= h^{4/3}p(h^{2/3}t); \\ p(x) &:= \left[(\xi_1'(x))^{-1/2} \right]'' (\xi_1'(x))^{-3/2} = \mathcal{O}(1 + |\xi_1(x)|)^{-2}. \end{aligned}$$

(In the last estimate, we have used the fact that $|V_1'(x)|^2 + |V_1''(x)| = \mathcal{O}((1 + |x|)^{-2})$, which is a consequence of Assumption (A2) and Cauchy estimates in Γ .) Defining \mathcal{K} as in (8.4), we reduce (8.8) to the Volterra equation,

$$(8.10) \quad f = \operatorname{Bi} + \mathcal{K}[Rf].$$

Then, a continuous solution of (8.10) will be solution of (8.8), too, and we expect it to have the right behavior at infinity. Moreover, it is enough to solve (8.10) separately on $\operatorname{Re} t \geq 0$ and $\operatorname{Re} t \leq 0$ (where, in any case, t remains on the curve $\Gamma := \{h^{-2/3}\xi_1(x); x \in [x_0, +\infty)\}$).

When $\operatorname{Re} t \geq 0$, one has $\operatorname{Bi}(t) \neq 0$, and we set $g := f/\operatorname{Bi}$. Then g must be solution to,

$$(8.11) \quad g = 1 + Lg,$$

with,

$$Lg(t) := \pi \int_0^t \left(\frac{\operatorname{Ai}(t)}{\operatorname{Bi}(t)} \operatorname{Bi}(s)^2 - \operatorname{Ai}(s)\operatorname{Bi}(s) \right) R(s)g(s)ds.$$

Using the asymptotic behaviours of Ai and Bi at infinity, and the fact that $\int_0^\infty (1+s)^{-1/2}(1+h^{2/3}s)^{-2}ds = \mathcal{O}(h^{-1/3})$, we see that $\|L\|_{C_b^0(\Gamma \cap \{\operatorname{Re} t \geq 0\})} = \mathcal{O}(h)$. Therefore, (8.11) can be solved by iteration on $\Gamma_+ := \Gamma \cap \{\operatorname{Re} t \geq 0\}$, and the corresponding solution to (8.10) satisfies,

$$f = \operatorname{Bi}(t)(1 + \mathcal{O}(h)) \text{ uniformly.}$$

On $\Gamma_- := \Gamma \cap \{\operatorname{Re} t \leq 0\}$, since $t = \mathcal{O}(h^{-2/3})$ there, and $|\operatorname{Ai}(s)| + |\operatorname{Bi}(s)| = \mathcal{O}((1 + |s|)^{-1/4})$ between 0 and t , we obtain

$$(1 + |t|)^{1/4} |\mathcal{K}[Rf](t)| = \mathcal{O}(h) \sup_{s \in \Gamma_-} (1 + |s|)^{1/4} |f(s)|,$$

and thus, (8.10) can be solved by iteration there, leading to a solution that satisfies,

$$f = \operatorname{Bi}(t) + \mathcal{O}(h(1 + |t|)^{-1/4}) \text{ uniformly.}$$

Moreover, the behaviour at infinity of f is obtained from that of Bi and of $\xi_1(x)$. This completes the proof of the proposition. \square

Remark 8.3. We also see on (8.11) that $g' = \mathcal{O}(h(1 + |t|)^{1/2})$. This leads to,

$$\begin{aligned} h^{2/3}(u_{1,R}^+)'(x) &= (\xi_1'(x))^{\frac{1}{2}} \text{Bi}'(h^{-\frac{2}{3}}\xi_1(x))(1 + \mathcal{O}(h)) \\ &\quad + \mathcal{O}(h^{2/3})(h^{2/3} + |\xi_1(x)|)^{1/2}(\xi_1'(x))^{-\frac{1}{2}} \text{Bi}(h^{-\frac{2}{3}}\xi_1(x)) \end{aligned}$$

on $[x_0, +\infty) \cap \{\text{Re } \xi_1(x) \geq 0\}$, and similar estimates are valid on $[x_0, +\infty) \cap \{\text{Re } \xi_1(x) \leq 0\}$, and for $h^{2/3}(u_{1,R}^-)'$, too. For instance, on $[x_0, +\infty) \cap \{\text{Re } \xi_1(x) \leq 0\}$, one obtains,

$$\begin{aligned} h^{2/3}(u_{1,R}^+)'(x) &= (\xi_1'(x))^{\frac{1}{2}} \text{Bi}'(h^{-\frac{2}{3}}\xi_1(x)) \\ &\quad + \mathcal{O}(h^{5/6})(1 + (h^{2/3} + |\xi_1(x)|)^{-1/4}); \\ (8.12) \quad h^{2/3}(u_{1,R}^-)'(x) &= 2(\xi_1'(x))^{\frac{1}{2}} \text{Ai}'(h^{-\frac{2}{3}}\xi_1(x)) \\ &\quad + \mathcal{O}(h^{5/6})(1 + (h^{2/3} + |\xi_1(x)|)^{-1/4}). \end{aligned}$$

Remark 8.4. Similar constructions can be done on $(-\infty, x_0]$, leading to solutions $u_{1,L}^\pm$ with the asymptotic behaviour,

$$u_{1,L}^\pm(x) \sim \frac{h^{\frac{1}{6}}}{\sqrt{\pi}} (V_1(x) - E)^{-1/4} e^{\mp \int_{x^*(E)}^x \sqrt{V_1(t) - E} dt/h} \quad (x \rightarrow -\infty),$$

where $x^*(E)$ is the only point near x^* where $V_1 - E$ vanishes.

Now, we treat the case $j = 2$. Here the situation is a bit different, because the set where $V_2 < 0$ is unbounded, and also because there is one turning point only. This actually permits us to directly obtain the asymptotic of the solutions both at $-\infty$ and at $+\infty$. We denote by $x_2(E)$ the unique point near 0 where $V_2 - E$ vanishes, and, when E is real, we set,

$$\begin{aligned} (8.13) \quad \xi_2(x; E) &= \left(\frac{3}{2} \int_{x_2(E)}^x \sqrt{E - V_2(t)} dt \right)^{\frac{2}{3}} \quad \text{when } x \geq x_2; \\ \xi_2(x; E) &= - \left(\frac{3}{2} \int_x^{x_2(E)} \sqrt{V_2(t) - E} dt \right)^{\frac{2}{3}} \quad \text{when } x \leq x_2. \end{aligned}$$

As before, we extend analytically this definition to complex values of E , and we have,

Proposition 8.5. Let $E \in \mathcal{D}_h(C_0)$. Then, there exist two real-valued solutions $u_{2,L}^\pm$ to equation $(P_2 - E)u = 0$ on \mathbb{R} , and two constants $a_2^\pm = 1 + \mathcal{O}(h)$, such that,

$$\begin{aligned} (8.14) \quad u_{2,L}^\pm(x) &\sim (1 + \mathcal{O}(h)) \frac{h^{\frac{1}{6}}}{\sqrt{\pi}} (V_2(x) - E)^{-1/4} e^{\mp \int_{x_2(E)}^x \sqrt{V_2(t) - E} dt/h} \quad (x \rightarrow -\infty); \\ (8.15) \quad &\frac{1}{2} a_2^- u_{2,L}^-(x) \pm i a_2^+ u_{2,L}^+(x) \\ &\sim (1 + \mathcal{O}(h)) \frac{h^{\frac{1}{6}}}{\sqrt{\pi}} (E - V_2(x))^{-1/4} e^{\mp i \int_{x_2(E)}^x \sqrt{E - V_2(t)} dt/h} \quad (x \rightarrow +\infty), \end{aligned}$$

uniformly with respect to $h > 0$ small enough, and,

$$u_{2,L}^-(x) = 2(\xi_2'(x))^{-\frac{1}{2}} \check{\text{Ai}}(h^{-\frac{2}{3}}\xi_2(x)) + \mathcal{O}(h(1+h^{-2/3}|\xi_2(x)|)^{-\frac{1}{4}}) \\ \text{on } \mathbb{R} \cap \{\text{Re } \xi_2(x) \geq 0\};$$

$$u_{2,L}^-(x) = 2(\xi_2'(x))^{-\frac{1}{2}} \check{\text{Ai}}(h^{-\frac{2}{3}}\xi_2(x))(1 + \mathcal{O}(h)) \text{ on } \mathbb{R} \cap \{\text{Re } \xi_2(x) \leq 0\};$$

$$u_{2,L}^+(x) = (\xi_2'(x))^{-\frac{1}{2}} \check{\text{Bi}}(h^{-\frac{2}{3}}\xi_2(x)) + \mathcal{O}(h(1+h^{-2/3}|\xi_2(x)|)^{-\frac{1}{4}}) \\ \text{on } \mathbb{R} \cap \{\text{Re } \xi_2(x) \geq 0\};$$

$$u_{2,L}^+(x) = (\xi_2'(x))^{-\frac{1}{2}} \check{\text{Bi}}(h^{-\frac{2}{3}}\xi_2(x))(1 + \mathcal{O}(h)) \text{ on } \mathbb{R} \cap \{\text{Re } \xi_2(x) \leq 0\},$$

uniformly as $h \rightarrow 0_+$.

Proof. The procedure is the same as for the previous proposition, but this time, setting $f(h^{-2/3}\xi_2(x)) := \xi_2'(x)^{\frac{1}{2}}u(x)$, the equation $(P_2 - E)u = 0$ becomes,

$$(8.16) \quad f''(t) + tf(t) = R(t)f(t),$$

where $R(t) = \mathcal{O}(h^{4/3}(1+h^{2/3}|t|)^{-2})$. In the case of $u_{2,L}^-$, we reduce (8.16) to the Volterra equation,

$$(8.17) \quad f = \check{\text{Ai}} + \tilde{\mathcal{K}}[Rf],$$

where $\tilde{\mathcal{K}}$ is defined by,

$$(8.18) \quad \tilde{\mathcal{K}}[f](t) := \int_{-\infty}^y K(-t, -s)f(s)ds.$$

In that case, we can follow the procedure of [24] on $\{\text{Re } \xi_2(x) \leq 0\}$, and obtain a solution with the required asymptotics (at $-\infty$ and for $h \rightarrow 0_+$). On the other hand, on $\Gamma_+ := \{\text{Re } \xi_2(x) \geq 0\}$, we rewrite (8.17) as,

$$f(t) = \check{\text{Ai}}(t) + \int_{-\infty}^0 K(-t, -s)R(s)f(s)ds + \tilde{\mathcal{K}}[Rf](t),$$

(where $\tilde{\mathcal{K}}$ is as in (8.4)), and the asymptotics at infinity of $\check{\text{Ai}}$ and $\check{\text{Bi}}$ give,

$$\tilde{\mathcal{K}}[Rf](t) = \mathcal{O}(h^{\frac{4}{3}}) \sup_{\Gamma_+} |f| \int_0^{|t|} (1+|t|)^{-\frac{1}{4}}(1+s)^{-\frac{1}{4}}(1+h^{\frac{2}{3}}s)^{-2}ds \\ = \mathcal{O}(h(1+|t|)^{-\frac{1}{4}}) \sup_{\Gamma_+} |f|.$$

In addition, (see also [24], Formula (3.18)), one has,

$$\int_{-\infty}^0 K(-t, -s)R(s)f(s)ds = \mathcal{O}\left(\frac{h^{\frac{4}{3}}}{(1+|t|)^{\frac{1}{4}}}\right) \sup_{\Gamma_+} |f| \int_0^\infty s^{-\frac{1}{2}}(1+h^{\frac{2}{3}}s)^{-2}ds \\ = \mathcal{O}(h(1+|t|)^{-\frac{1}{4}}) \sup_{\Gamma_+} |f|.$$

Thus, (8.17) can be solved by iteration on Γ_+ , too, and there the solution satisfies,

$$f(t) = \check{\text{Ai}}(t) + \mathcal{O}(h(1+|t|)^{-\frac{1}{4}}).$$

The result for $u_{2,L}^-$ follows by taking $u_{2,L}^-(x) := 2(\xi_2'(x))^{-1/2}f(h^{-2/3}\xi_2(x))$.

In the case of $u_{2,L}^+$, we reduce (8.16) to the Volterra equation,

$$(8.19) \quad f = \check{\text{Bi}} + \tilde{\mathcal{K}}[Rf].$$

First working on $\{\text{Re } t \leq 0\}$, the same procedure as for Proposition 8.2 leads to a solution that satisfies $f = (1 + \mathcal{O}(h))\check{\text{Bi}}$. Next, on $\{\text{Re } t \geq 0\}$, the result follows exactly as for $u_{2,L}^-$, but this time there is no need to rewrite the Volterra equation.

The asymptotic of each solution at $-\infty$ follows from that of Ai and Bi , and the fact that $\xi_2(x) \sim cx^{2/3}$ at $+\infty$ (with $c > 0$ constant).

Finally, since $\check{\text{Ai}} \pm i\check{\text{Bi}}$ do not vanish on \mathbb{R} , by setting $g := f/(\check{\text{Ai}} \pm i\check{\text{Bi}})$, we see (e.g. as in the proof of Proposition 8.2) that there exist two solutions f_{\pm} to (8.16) on \mathbb{R}_+ satisfying $f_{\pm} = (1 + \mathcal{O}(h))(\check{\text{Ai}} \pm i\check{\text{Bi}})$. They give rise to two solutions v_{\pm} to $(P_2 - E)v = 0$ (that are conjugated of each other for real values of E) and by computing their Wronskians with $u_{2,L}^{\pm}$, we see that they are of the form $v_{\pm} = \frac{1}{2}a_2^- u_{2,L}^- \pm ia_2^+ u_{2,L}^+$ with $a_2^{\pm} = 1 + \mathcal{O}(h)$, so that (8.15) follows, too. \square

Remark 8.6. Here again, estimates on $h^{2/3}(u_{2,L}^{\pm})'$ can also be derived from the construction (see Remark 8.3).

Remark 8.7. Near infinity, all these constructions extend to a complex sector in x , with the same asymptotic behaviours as on the real.

Remark 8.8. These constructions can also be adapted to a problem on \mathbb{R}_+ (e.g., for radial solutions of a problem in \mathbb{R}^n), with potential $V_j(r)$ ($j = 1, 2$) behaving like c_j/r^{α} , with $c_j > 0$ constant and $0 \leq \alpha < 2$, as $r \rightarrow 0_+$. In this case, $-\infty$ is replaced by $r = 0$, and the decaying solutions at $-\infty$ become solutions vanishing at 0. Thus, in the construction of $u_{j,L}^-$ ($j = 1, 2$), it is enough to replace $\check{\text{Ai}}$ (for instance in (8.17)) by a linear combination $\check{\text{Ai}} + \alpha_j \check{\text{Bi}}$, where $\alpha_j \in \mathbb{R}$ is chosen in such a way that $\check{\text{Ai}}(-h^{-2/3}\xi_j(0)) + \alpha_j \check{\text{Bi}}(-h^{-2/3}\xi_j(0)) = 0$ (here $\xi_j(r)$ is the corresponding change of variable similar to (8.13)), and to use a fundamental solution of the Airy equation vanishing at $-h^{-2/3}\xi_j(0)$ (e.g., in (8.18), one must replace $-\infty$ by $-h^{-2/3}\xi_j(0)$). Then the proof proceeds exactly in the same way.

For potentials behaving like c_j/r^2 at 0 (with $c_j = c_j(h) > 0$), the adaptation is even simpler since, in that case, $\xi_j(r) \rightarrow -\infty$ as $r \rightarrow 0_+$, so that the construction remains the same.

8.3. Formulae.

$$\begin{aligned}
u_{1,R}^+ &\sim (\xi_1')^{-\frac{1}{2}} \text{Bi}(h^{-\frac{2}{3}} \xi_1) \sim \text{Bi}(y - \rho) \\
u_{1,R}^- &\sim 2(\xi_1')^{-\frac{1}{2}} \text{Ai}(h^{-\frac{2}{3}} \xi_1) \sim 2\text{Ai}(y - \rho) \\
u_{2,L}^+ &\sim (\xi_2')^{-\frac{1}{2}} \check{\text{Bi}}(h^{-\frac{2}{3}} \xi_2) \sim \check{\text{Bi}}(y + \rho) \\
u_{2,L}^- &\sim 2(\xi_2')^{-\frac{1}{2}} \check{\text{Ai}}(h^{-\frac{2}{3}} \xi_2) \sim 2\check{\text{Ai}}(y + \rho) \\
u_{1,L}^+ &\sim \frac{1}{2} \left(\cos \frac{\mathcal{A}}{h} \right) u_{1,R}^- - \left(\sin \frac{\mathcal{A}}{h} \right) u_{1,R}^+ \\
u_{1,L}^- &\sim \left(\sin \frac{\mathcal{A}}{h} \right) u_{1,R}^- + 2 \left(\cos \frac{\mathcal{A}}{h} \right) u_{1,R}^+ \\
u_{2,R}^+ &\sim \sqrt{2} e^{i\pi/4} \left(\frac{1}{2} u_{2,L}^- + i u_{2,L}^+ \right) \\
u_{2,R}^- &\sim \frac{1}{\sqrt{2}} e^{i\pi/4} \left(\frac{1}{2} u_{2,L}^- - i u_{2,L}^+ \right) \\
\widetilde{\mathcal{W}}(u_{j,L}^-, u_{j,L}^+) &\sim \frac{-2}{\pi} \quad ; \quad \widetilde{\mathcal{W}}(u_{j,R}^-, u_{j,R}^+) \sim \frac{2}{\pi} \\
\widetilde{\mathcal{W}}(u_{1,L}^-, u_{1,R}^-) &\sim \frac{-4}{\pi} \cos \frac{\mathcal{A}}{h} \quad ; \quad \widetilde{\mathcal{W}}(u_{2,L}^-, u_{2,R}^-) \sim \frac{i\sqrt{2}}{\pi} e^{i\frac{\pi}{4}} \\
\widetilde{\mathcal{W}}(u_{1,L}^\pm, u_{1,R}^\mp) &= \frac{2}{\pi} \sin \frac{\mathcal{A}}{h} \\
\widetilde{\mathcal{W}}(u_{2,L}^-, u_{2,R}^+) &\sim \frac{-2i\sqrt{2}}{\pi} e^{i\frac{\pi}{4}} \quad ; \quad \widetilde{\mathcal{W}}(u_{2,L}^+, u_{2,R}^-) \sim \frac{1}{\pi\sqrt{2}} e^{i\frac{\pi}{4}}
\end{aligned}$$

Acknowledgements A. Martinez was partially supported by Ritsumeikan University, where the final part of this work was done, and he would like to thank the Mathematical Department of this University for his warm hospitality between April and July 2015. In addition, S. Fujiié and T. Watanabe thank JSPS for its financial support, and the Department of Mathematics of the University of Bologna where part of this work was done.

REFERENCES

- [1] J. Aguilar, J.M. Combes: *A class of analytic perturbations for one-body Schrödinger Hamiltonians*. Comm. Math. Phys., 22 (1971), no. 4, 269–279.
- [2] H. Baklouti: *Asymptotique des largeurs de résonances pour un modèle d'effet tunnel microlocal*. Ann. Inst. H. Poincaré Phys. Theor., 68 (1998); no. 2, 179–228.
- [3] M. Dimassi, S. Sjöstrand: *Spectral Asymptotics in the Semi-Classical Limit*. Cambridge University Press, 1999.
- [4] S. Dyatlov, M. Zworski: *Mathematical theory of scattering resonances*. Book in progress, <http://math.mit.edu/~dyatlov/res/res.pdf>
- [5] S. Fujiié, A. Lahamar-Benbernou, A. Martinez: *Width of shape resonances for non globally analytic potentials*. J. Math. Soc. Japan, 63 (2011), no. 1, 1–78.
- [6] S. Fujiié, C. Lasser, L. Nédélec: *Semiclassical resonances for a two-level Schrödinger operator with a conical intersection*. Asympt. Anal., 65 (2009), no. 1–2, 17–58.
- [7] S. Fujiié, T. Ramond: *Matrice de scattering et résonances associées à une orbite hétérocline*. Ann. Inst. H. Poincaré Phys. Theor., 69 (1998), no. 1, 31–82.
- [8] A. Grigis, A. Martinez: *Resonance widths in a case of multidimensional phase space tunneling*. Asymptot. Anal., 91 (2015), no. 1, 33–904.
- [9] A. Grigis, A. Martinez: *Resonance widths for the molecular predissociation*. Anal. PDE, 7 (2014), no. 5, 1027–1055.

- [10] E.M. Harrell: *General lower bounds for resonances in one dimension*. Comm. Math. Phys., 86 (1982), no. 2, 221-225.
- [11] B. Helffer, A. Martinez: *Comparaison entre les diverses notions de résonances*. Helv. Phys. Acta, 60 (1987), no. 8, 992-1003.
- [12] B. Helffer, J. Sjöstrand: *Résonances en limite semiclassique*. Bull. Soc. Math. France, Mémoire No. 24-25, 1986.
- [13] P. Hislop, I.M. Sigal: *Introduction to Spectral Theory. With Applications to Schrödinger Operators*. Applied Mathematical Sciences, 113. Springer-Verlag, New York, 1996.
- [14] M. Klein: *On the mathematical theory of predissociation*. Ann. Physics, 178 (1987), no. 1, 48-73.
- [15] M. Klein, A. Martinez, R. Seiler, X.W. Wang: *On the Born-Oppenheimer expansion for polyatomic molecules*. Comm. Math. Physics, 143 (1992), no. 3, 607-639.
- [16] A. Martinez: *An Introduction to Semiclassical and Microlocal Analysis*. Springer-Verlag New-York, UTX Series, 2002.
- [17] A. Martinez, P. Briet: *Estimates on the molecular dynamics for the pre dissociation process*. Preprint 2015. <http://arxiv.org/abs/1503.05507>
- [18] A. Martinez: *Estimates on Complex Interactions in Phase Space*. Math. Nachr., 167 (1994), p.203-254.
- [19] A. Martinez, B. Messirdi: *Resonances for Diatomic Molecules in the Born-Oppenheimer Approximation*. Comm. Partial Differential Equations, 19 (1994), no. 7-8, 1139-1162.
- [20] A. Martinez, V. Sordani: *Twisted pseudodifferential calculus and application to the quantum evolution of molecules*. Mem. Amer. Math. Soc., 200 (2009), no. 936.
- [21] S. Nakamura: *On an example of phase-space tunneling*. Ann. Inst. H. Poincaré Phys. Theor., 63 (1995), no. 2, 211-229.
- [22] M. Reed, B. Simon: *Methods of Modern Mathematical Physics, Vol. I-IV*, Academic Press New York, 1972.
- [23] A. Voros: *The return of the quartic oscillator: the complex WKB method*. Ann. Inst. H. Poincaré Sect. A, 39 (1983), no. 3, 211-338.
- [24] D.R. Yafaev: *The semiclassical limit of eigenfunctions of the Schrödinger equation and the Bohr-Sommerfeld quantization condition, revisited*. Algebra i Analiz, 22 (2010), no. 6, 270-291; translation in St. Petersburg Math. J., 22 (2011), no. 6, 1051-1067.
- [25] M. Zworski: *Semiclassical Analysis, Graduate Studies in Mathematics, 138*. American Mathematical Soc., 2012.