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ACCURATE WKB APPROXIMATION FOR A 1D PROBLEM WITH LOW REGULARITY

F. Nier

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Abstract. This article is concerned with the analysis of the WKB expansion in a classically forbidden region for a one dimensional boundary value Schrodinger equation with a non smooth potential. The assumed regularity of the potential is the one coming from a non linear problem and seems to be the critical one for which a good exponential decay estimate can be proved for the first remainder term. The treatment of the boundary conditions brings also some interesting subtleties which require a careful application of Carleman's method.

1. Introduction. In the analysis of $1D$ out-of-equilibrium Schrödinger-Poisson systems, which arise in the modelling of quantum electronic devices like resonant tunneling diodes, one part of the analysis ends with some accurate WKB-approximation with singular potentials. The complete presentation of the nonlinear problem with proper references is provided in [2], [3]. The numerical

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applications of the derived reduced model to the realistic simulation of quantum electronic devices have been shown in [1].

This article provides a complete proof of Proposition 8.2 in [3], which is standard for smooth potentials but requires some adaptation within the framework of the nonlinear problem. As we shall see, the assumed regularity of the potential, which is exactly the one provided from the a priori estimates in the nonlinear $1D$ Schrödinger-Poisson problem, seems to be just enough in order to get an effective comparison with a WKB approximation. Besides, this rather simple problem provides a good pedagogical example for the analysis of exponentially small quantities and the application of Carleman's method : As a $1D$-problem its geometrical presentation is significantly simplified, while the weak regularity and the boundaries bring some interesting subtleties (see Section 3 after the proof for a summary).

We refer the reader to [5] or [4] for a presentation of the general method and to [6] for the treatment along a boundary for some specific multidimensional boundary value problem.

Here are the data of the problem

- $[a,b]$ is a real interval $a<b$.
- B is a positive constant.
- $(\tilde{\mathcal{V}}_h)_{h\in(0,h_0)}$, $h_0>0$, is a family of real-valued potentials with uniformly bounded second derivative as a bounded measure on $[a,b]$

$$\left|\tilde{\mathcal{V}}_h(a)\right|+\left|\tilde{\mathcal{V}}_h(b)\right|+\left\|\tilde{\mathcal{V}}_h''\right\|_{\mathcal{M}_b([a,b])}\leq C$$

  and which satisfies the uniform lower bound

$$\inf_{h\in(0,h_0),x\in I}\tilde{\mathcal{V}}_h(x)=:\Lambda_0>0.$$

- k is a positive parameter which can be related with h but with the constraints

$$k\in[k_0,\sqrt{\Lambda_0}],$$

  for some $k_0>0$ independent of h.

We shall consider the boundary value problem

$$(1.1)\qquad \begin{cases} \left(-h^2\partial_x^2 + \tilde{\mathcal{V}}_h - k^2\right)\psi_h = 0 \\ h\psi_h'(a) + ik\psi_h(a) = 2ike^{i\frac{ka}{h}} \\ h\psi_h'(b) - i\sqrt{k^2+B}\psi_h(b) = 0, \end{cases}$$

equivalent to a $1D$-scattering problem after introducing the k-dependent transparent boundary conditions.

2. Result. The Agmon distance for our $1D$ problem has a simple definition.

Definition 2.1. *For $k^2 \in (0, \Lambda_0)$, the distance $\tilde{d}_h$ on $[a,b]$ is defined by*

$$(2.1)\qquad \tilde{d}_h(x,y) = \left| \int_x^y \sqrt{(\tilde{\mathcal{V}}_h(t) - k^2)}\ dt \right|.$$

The first-order WKB-approximation of the solution ψ_h to (1.1) is

$$(2.2)\qquad \psi_{app,h}(k,x) = (\tilde{\mathcal{V}}_h(x) - k^2)^{-1/4}\left[C_-(k)e^{-\tilde{d}_h(a,x)/h} + C_+(k)e^{\tilde{d}_h(a,x)/h}\right]$$

where $(C_-(k), C_+(k))$ solves the system

$$(2.3)\qquad \begin{cases} \left[-(\tilde{\mathcal{V}}_h(a) - k^2)^{1/2} + ik\right]C_-(k) = 2ike^{i\frac{ka}{h}}\left(\tilde{\mathcal{V}}_h(a) - k^2\right)^{1/4}, \\ \left[-(\tilde{\mathcal{V}}_h(b) - k^2)^{1/2} - i\sqrt{k^2+B}\right]C_-(k) \\ \qquad + \left[\left(\tilde{\mathcal{V}}_h(b) - k^2\right)^{1/2} - i\sqrt{k^2+B}\right]\left(C_+(k)e^{2\frac{\tilde{d}_h(a,b)}{h}}\right) = 0. \end{cases}$$

Theorem 2.2. *The previous assumptions on $\tilde{\mathcal{V}}_h$, B and k imply*

$$(2.4)\qquad \lim_{h\to 0}\left\| e^{\frac{\tilde{d}_h(a,.)}{h}}\left(\psi_h - \psi_{app,h}\right)\right\|_{L^\infty([a,b])} = 0.$$

Proof. We start our proof with two remarks:

a) It suffices to prove the convergence (2.4) for any subsequence $(h_n)_{n\to\infty}$ with $\lim_{n\to\infty} h_n = 0$. Hence any compactness condition can be transformed into a convergence assumption. For example the uniform boundedness $\tilde{\mathcal{V}}_h''$ in $\mathcal{M}_b([a,b])$, can be replaced by a weak convergence assumption (after extracting a subsequence).

b) The potential $\tilde{\mathcal{V}}_h$ can be replaced by V_h according to

$$V_h\Big|_{[a,b-h(\log h)^2]} = \tilde{\mathcal{V}}_h\Big|_{[a,b-h(\log h)^2]} \quad \text{and} \quad V_h'' = \tilde{\mathcal{V}}_h'' 1_{[a,b-h(\log h)^2]}. \tag{2.5}$$

Indeed such a variation implies

$$\left|V_h'(x) - \tilde{\mathcal{V}}_h'(x)\right| \leq C 1_{[b-h(\log h)^2,b]}(x)$$

$$\left|V_h(x) - \tilde{\mathcal{V}}_h(x)\right| \leq Ch(\log h)^2 1_{[b-h(\log h)^2,b]}(x)$$

$$\left|d_h(a,x) - \tilde{d}_h(a,x)\right| \leq Ch^2(\log h)^4$$

$$\text{by setting} \qquad d_h(a,x) = \int_a^x \sqrt{V_h(t) - k^2}\; dt.$$

Hence the result for $\tilde{\mathcal{V}}_h$, which involves only the distance $h^{-1}\tilde{d}_h$ and the potential $\tilde{\mathcal{V}}_h$, can be deduced from the result for V_h. Indeed the variation of $\psi_{app,h}$ due to this change of potential is easily checked to be $o(h^0)$ while the same result for ψ_h is done in Lemma 2.3 below.

Hence we can assume

$$\tilde{\mathcal{V}}_h''\Big|_{]b-h(\log h)^2,b]} \equiv 0 \quad \text{and} \quad \tilde{\mathcal{V}}_h'' \overset{h\to 0}{\rightharpoonup} \mu_0 \text{ in } \mathcal{M}_b([a,b]).$$

We shall set for convenience

$$\varphi(x) = \tilde{d}_h(x,a) = \int_a^x \sqrt{\tilde{\mathcal{V}}_h(t) - k^2}\; dt,$$

where the h-dependence does not appear any more in the simplified notation $\varphi(x)$.

The process starts like the standard WKB approximation with regular potentials. Consider the ansatz

$$\psi = \alpha_-(x,h)e^{-\frac{\varphi(x)}{h}} + \alpha_+(x,h)e^{+\frac{\varphi(x)}{h}},$$

$$\text{with} \qquad \alpha_\pm(x,h) = \alpha_{0,\pm}(x) + h\alpha_{1,\pm}(x),$$

and compute

$$\left[-h^2\partial_x^2+\tilde{\mathcal{V}}_h(x)-k^2\right]\psi=\Big[-h^2\alpha_-''+2h(\varphi')^{1/2}[(\varphi')^{1/2}\alpha_-]'$$

$$+\left(-h^2\alpha_+''-2h(\varphi')^{1/2}[(\varphi')^{1/2}\alpha_+]'\right)e^{\frac{2\varphi}{h}}\Big]e^{-\frac{\varphi}{h}} \tag{2.6}$$

$$h\psi'(a)+ik\psi(a)=(h\alpha_-'(a)+(-\varphi'(a)+ik)\alpha_-(a))$$

$$+(h\alpha_+'(a)+(\varphi'(a)+ik)\alpha_+(a)) \tag{2.7}$$

$$h\psi'(b)-i\sqrt{k^2+B}\psi(b)=(h\alpha_-'(b)+(-\varphi'(b)-i\sqrt{k^2+B})\alpha_-(b))e^{-\frac{\varphi(b)}{h}}$$

$$+(h\alpha_+'(b)+(\varphi'(b)-i\sqrt{k^2+B})\alpha_+(b))e^{+\frac{\varphi(b)}{h}}. \tag{2.8}$$

We make the main term of every right-hand side vanish. By noticing that a solution to $[(\varphi')^{1/2}\alpha_\pm]'=0$ writes

$$\alpha_\pm(x)=C_\pm(\varphi')^{-1/2}(x)=\frac{C_\pm}{\left(\tilde{\mathcal{V}}_h(x)-k^2\right)^{1/4}},$$

one is led to consider the linear system

$$\begin{cases}(-\varphi'(a)+ik)C_-=b_1\\ (-\varphi'(b)-i\sqrt{k^2+B})C_-+(\varphi'(b)-i\sqrt{k^2+B})\left(C_+e^{\frac{2\varphi(b)}{h}}\right)=b_2.\end{cases} \tag{2.9}$$

We now consider the approximation

$$\psi_{app,h}=\psi_0+h\psi_1$$

of which the terms are constructed as follows. In Theorem 2.2, the function $\psi_{app,h}$ is defined without the correction term $h\psi_1$. This will not change the final result because the L^∞-norm of ψ_1 will be $\mathcal{O}(1)$.

The first term equals

$$\psi_0=a_{0-}(x)e^{-\frac{\varphi(x)}{h}}+a_{0+}(x)e^{\frac{\varphi(x)}{h}}=\frac{C_{0-}}{(\tilde{\mathcal{V}}_h(x)-k^2)^{1/4}}e^{-\frac{\varphi(x)}{h}}+\frac{C_{0+}}{(\tilde{\mathcal{V}}_h(x)-k^2)^{1/4}}e^{\frac{\varphi(x)}{h}},$$

where (C_{0-}, C_{0+}) solve the system (2.9) with $b_1 = 2ike^{i\frac{ka}{h}}\left(\tilde{\mathcal{V}}_h(a) - k^2\right)^{1/4}$ and $b_2 = 0$.

Before introducing the second term, consider a cut-off function $\chi \in \mathcal{C}_0^\infty(]1,2[)$ with $\int \chi = 1$ and take

$$\chi_h(x) = \frac{1}{h\,|\log h|}\chi(\frac{x}{h\,|\log h|}) \quad x \in \mathbb{R}.$$

The function ψ_1 is the sum of two terms

$$\psi_1 = (a_{1-} + a_{b-})\, e^{-\frac{\varphi}{h}} + (a_{1+} + a_{b+})\, e^{\frac{\varphi}{h}}$$

where $a_{1\pm}$ solves the Cauchy problem

$$\text{(2.10)} \qquad \begin{cases} 2(\varphi')^{1/2}\left((\varphi')^{1/2}a_{1\pm}\right)' = \mp\chi_h * \left(1_{[a,b-10h|\log h|]}a''_{0\pm}\right) \\ a_{1-}(a) = 1, \quad a_{1+}(a) = e^{-\frac{2\varphi(b)}{h}}, \end{cases}$$

with simple initial conditions at $x = a$, while the proper boundary values are taken into account with the correction term $a_{b\pm}$. This term, $a_{b\pm}$, equals $\dfrac{C_{b\pm}}{\left(\tilde{\mathcal{V}}_h(x)) - k^2\right)^{1/4}}$ where the pair (C_{b-}, C_{b+}) solves the system (2.9) with

$$\begin{aligned} \frac{b_1}{\left(\tilde{\mathcal{V}}_h(a) - k^2\right)^{1/4}} &= a'_{0-}(a) + a'_{0+}(a) - (-\varphi'(a) + ik) - \left[(\varphi'(a) + ik)e^{-\frac{2\varphi(b)}{h}}\right] \\ \frac{b_2}{\left(\tilde{\mathcal{V}}_h(b) - k^2\right)^{1/4}} &= a'_{0-}(b) + a'_{0+}(b)e^{\frac{2\varphi(b)}{h}} - (-\varphi'(b) - i\sqrt{k^2+B})a_{1-}(b) \\ &\qquad - (\varphi'(b) - i\sqrt{k^2+B})\left(a_{1+}(b)e^{\frac{2\varphi(b)}{h}}\right). \end{aligned}$$

For $h \in (0, h_0)$, the right-hand side of (2.10) belongs to $\mathcal{C}_0^\infty(]a,b[)$ and the boundary value problems (2.10) admit $\mathcal{C}^1$ classical solutions $a_{1\pm}$.

For such an ansatz, set

$$u := \psi_{app,h} - \psi_h$$

and compute with the help of (2.6), (2.7), (2.8)

$$\left(-h^2\partial_x^2+\tilde{\mathcal{V}}_h-k^2\right)u=\left(-h^2r_0+h^2r_{0h}-h^3r_1\right)e^{-\frac{\varphi}{h}} \tag{2.11}$$

$$hu'(a)+iku(a)=h^2\varrho(a)+\mathcal{O}(e^{-\frac{2\varphi(b)}{h}}) \tag{2.12}$$

$$hu'(b)-i\sqrt{k^2+B}u(b)=h^2\varrho(b)e^{-\frac{\varphi(b)}{h}}, \tag{2.13}$$

after introducing the notations

$$\begin{aligned}
r_0 &= a''_{0-}+a''_{0+}e^{\frac{2\varphi}{h}},\\
r_{0h} &= \chi_h*(1_{[a,b-10h|\log h|]}a''_{0-})+(\chi_h*(1_{[a,b-10h|\log h|]}a''_{0+})e^{\frac{2\varphi}{h}})\\
r_1 &= a''_{1-}+a''_{b-}+(a''_{1+}+a''_{b+})e^{\frac{2\varphi}{h}}\\
\varrho(t) &= a'_{1-}(t)+a'_{b-}(t)+(a'_{1+}(t)+a'_{b+}(t))e^{\frac{2\varphi}{h}}.
\end{aligned}$$

The identities

$$\begin{aligned}
a'_{0\pm} &= -\frac{C_{0\pm}}{4}\frac{\tilde{\mathcal{V}}'_h}{(\tilde{\mathcal{V}}_h-k^2)^{5/4}} \quad \text{and}\\
a''_{0\pm} &= C_{0\pm}\left[\tfrac{5}{16}\tfrac{(\tilde{\mathcal{V}}'_h)^2}{(\tilde{\mathcal{V}}_h-k^2)^{9/4}}-\tfrac{1}{4}\tfrac{\tilde{\mathcal{V}}''_h}{(\tilde{\mathcal{V}}_h-k^2)^{5/4}}\right],
\end{aligned} \tag{2.14}$$

lead to the estimates

$$\begin{aligned}
&\left\|a'_{1-}\right\|_{\mathcal{M}_b}+\|a_{1-}\|_{L^\infty}+e^{\frac{2\varphi(b)}{h}}\left\|a'_{1+}\right\|_{\mathcal{M}_b}+e^{\frac{2\varphi(b)}{h}}\|a_{1+}\|_{L^\infty}=\mathcal{O}(1)\\
&\left\|a''_{1-}\right\|_{\mathcal{M}_b}+\left\|a'_{1-}\right\|_{L^\infty}+e^{\frac{2\varphi(b)}{h}}\left\|a''_{1+}\right\|_{\mathcal{M}_b}+e^{\frac{2\varphi(b)}{h}}\left\|a'_{1+}\right\|_{L^\infty}=\mathcal{O}\left(\frac{1}{h\,|\log h|}\right).
\end{aligned}$$

Meanwhile, the computation of (C_{b-},C_{b+}) imply

$$\begin{aligned}
&\|a_{b-}\|_{L^\infty}+\|a'_{b-}\|_{L^\infty}+\|a''_{b-}\|_{\mathcal{M}_b}\\
&\qquad\qquad+e^{\frac{2\varphi(b)}{h}}\left(\|a_{b+}t\|_{L^\infty}+\|a'_{b+}\|_{L^\infty}+\|a''_{b+}\|_{\mathcal{M}_b}\right)=\mathcal{O}(1).
\end{aligned}$$

Hence the above quantities r_0, r_{0h}, r_1 and $\varrho(t)$ satisfy

$$\|r_0\|_{\mathcal{M}_b} = \mathcal{O}(1), \quad \|r_{0h}\|_{\mathcal{M}_b} = \mathcal{O}(1),$$
$$\|r_1\|_{\mathcal{M}_b} = \mathcal{O}\left(\frac{1}{h\,|\log h|}\right),$$
$$|\varrho(a)| + |\varrho(b)| = \mathcal{O}\left(\frac{1}{h\,|\log h|}\right).$$

The identity (A.1) with $u_1 = u_2 = \psi_{app,h} - \psi_h$ and $v_1 = v_2 = v = e^{\frac{\theta}{h}} u$ reads

$$\begin{aligned}(2.15)\quad & h^2 \int_a^b e^{\frac{\theta-\varphi}{h}} \left(-r_0 + r_{0h} - hr_1\right) \overline{v}\, dx \\ &= \int_a^b \left|hv'\right|^2\, dx + \int_a^b \left(\tilde{\mathcal{V}}_h - k^2 - (\theta')^2\right) |v|^2\, dx \\ &+ h \int_a^b \theta'(v'\overline{v} - v\overline{v'})\, dx - he^{\frac{2\theta(a)}{h}}(ik)\,|u(a)|^2 - he^{\frac{2\theta(b)}{h}} i\sqrt{k^2+B}\,|u(b)|^2 \\ &+ h^3 \left[e^{\frac{\theta(a)}{h}} \varrho(a)\overline{v}(a) - e^{\frac{\theta(b)-\varphi(b)}{h}} \varrho(b)\overline{v}(b)\right].\end{aligned}$$

a) Take first $\theta = 0$. The equality of the real parts of both sides imply $\|hu'\|_{L^2} + \|u\|_{L^2} = \mathcal{O}(1)$, while the imaginary parts satisfy

$$\begin{aligned} h^2\,\mathcal{I}\mathrm{m} \int_a^b (-r_0 + r_{0h} - hr_1) e^{\frac{-\varphi}{h}} \overline{u} &= -hk\,|u(a)|^2 - h\sqrt{k^2+B}\,|u(b)|^2 \\ &+ h^3\,\mathcal{I}\mathrm{m}\left[\varrho(a)\overline{u}(a) - e^{-\frac{\varphi(b)}{h}} \varrho(b)\overline{u}(b)\right].\end{aligned}$$

This implies

$$|u(a)| = \mathcal{O}\left(h^{1/2}\,|\log h|^{-\frac{1}{2}}\right).$$

b) Take now $\theta = \varphi$. The real parts satisfy

$$h^2\,\mathbb{R}\mathrm{e} \int_a^b (-r_0 + r_{0h} - hr_1)\,\overline{v}\, dx = \int_a^b \left|hv'\right|^2\, dx + h^3\,\mathbb{R}\mathrm{e}\left[\varrho(a)\overline{v}(a) - \varrho(b)\overline{v}(b)\right].$$

By using $\|-r_0 + r_{0h}\|_{\mathcal{M}_b} = \mathcal{O}(1)$, one gets

$$\left\|v'\right\|_{L^2} = \mathcal{O}(1)$$

and owing to $v(a) = u(a) = \mathcal{O}(h^{1/2}\,|\log h|^{-\frac{1}{2}})$, the estimate

$$|v(a)| + |v(b)| + \left\|v'\right\|_{L^2} + \|v\|_{L^2} = \mathcal{O}(1) \tag{2.16}$$

c) Take again $\theta = \varphi$. In order to transform the estimate $\|v\|_{L^\infty} = \mathcal{O}(1)$ into $\|v\|_{L^\infty} = o(h^0)$, consider more carefully the term

$$\begin{aligned} h^2\,\mathrm{Re}\int_a^b (-r_0 + r_{0h} - hr_1)\overline{v}\;dx &= h^2\,\mathrm{Re}\int_a^b \left[-r_0 1_{[a,b-10h|\log h|]}(x) + r_{0h}\right]\overline{v}\;dx \\ &\quad + \mathcal{O}\left(h^2\left|\int_{b-10h|\log h|}^b r_0\overline{v}\;dx\right|\right) + \mathcal{O}\left(h^2\,|\log h|^{-1}\right). \end{aligned}$$

The aim is to prove that it is an $o(h^2)$ as $h \to 0$.

Here we use the assumption $\tilde{\mathcal{V}}_h'' \equiv 0$ on $[b-h(\log h)^2, b] \supset [b-10h|\log h|, b]$, made after the initial reduction. Indeed the expression $r_0 = a_{0-}'' + a_{0+}'' e^{\frac{2\varphi}{h}}$ and the second formula of (2.14) imply that r_0 is a uniformly bounded Lipschitz function on $[b-10h|\log h|, b]$ and

$$\mathcal{O}\left(h^2\left|\int_{b-10h|\log h|}^b r_0\overline{v}\;dx\right|\right) = \mathcal{O}\left(h^3\,|\log h|\right).$$

The estimate $\|v\|_{L^2} + \|v'\|_{L^2} = \mathcal{O}(1)$ given by (2.16) and the compact embedding $H^1(]a,b[) \subset \mathcal{C}^0([a,b])$, allows to add the assumption

$$\lim_{h\to 0} v = v^0 \quad \text{in } \mathcal{C}^0([a,b]).$$

This leads to

$$\begin{aligned} &h^2\,\mathrm{Re}\int_a^b (-r_0 1_{[a,b-10h|\log h|]}(x) + r_{0h})\overline{v}\;dx \\ &\qquad = h^2\,\mathrm{Re}\int_a^b (-r_0 1_{[a,b-10h|\log h|]}(x) + r_{0h})\overline{v^0}\;dx + h^2\mathcal{O}\left(\left\|v - v^0\right\|_{L^\infty}\right). \end{aligned}$$

But the definition

$$r_{0h} = \chi_h * (1_{[a,b-10h|\log h|]}(x) r_0)$$

ensures that the first term of the right-hand side is an $o(h^2)$ as $h \to 0$. Indeed the fact that the mass of the measure $r_0 1[a, b-10h|\log h|]$ in the interval $]b -$

$10h|\log h|, b]$ and the support condition $\operatorname{supp}\chi_h \subset [h|\log h|, 2h|\log h|]$, ensure the weak convergence applied with the fixed test function $v^0 \in \mathcal{C}^0([a,b])$.

After possibly extracting a subsequence, the real part of (2.15) with $\theta = \varphi$ leads to

$$\lim_{h\to 0} \left\|v'\right\|_{L^2} + |v(a)| = 0.$$

This ends the proof. $\square$

Lemma 2.3. *Let V_h be the modified version of the potential $\tilde{\mathcal{V}}_h$, $h \in (0, h_0)$, with a truncated second derivative according to (2.5). Let ψ_h and $\tilde{\psi}_h$ denote the solutions to the boundary value problem (1.1) with the potentials V_h and $\tilde{\mathcal{V}}_h$ respectively. Then the difference $\psi_h - \tilde{\psi}_h$ satisfies*

$$\lim_{h\to 0} \left\| e^{\frac{\varphi}{h}} (\psi_h - \tilde{\psi}_h) \right\|_{L^\infty([a,b])} = 0,$$

where $\varphi(x)$ is any of the Agmon distances $\tilde{d}_h(a,x)$ or $d_h(a,x)$.

P r o o f. Let $\varphi(x)$ and $\tilde{\varphi}(x)$ denote respectively the Agmon distance $d_h(a,x)$ and $\tilde{d}_h(a,x)$. They satisfy

$$|\varphi(x) - \tilde{\varphi}(x)| = \mathcal{O}(h^2(\log h)^4).$$

Thus the exponential weights $e^{\varphi/h}$ and $e^{\tilde{\varphi}/h}$ are uniformly equivalent.

The result of Theorem 2.2 holds for the truncated potential V_h and this implies

$$\left\| e^{\frac{\varphi}{h}} \psi_h \right\|_{L^\infty([a,b])} = \mathcal{O}(1),$$

since such an estimate is obviously true for the WKB approximation.

The difference $u = \tilde{\psi}_h - \psi$ solves the boundary value problem

$$\begin{cases} \left(-h^2\partial_x^2 + \tilde{\mathcal{V}}_h - k^2\right) u = \left(\tilde{\mathcal{V}}_h - V_h\right) \psi_h =: f_h \\ hu'(a) + iku(a) = 0 \\ hu'(b) - i\sqrt{k^2+B}\,u(b) = 0, \end{cases}$$

The estimate

$$\left| V_h(x) - \tilde{\mathcal{V}}_h(x) \right| \leq Ch(\log h)^2 1_{[b-h(\log h)^2, b]}(x)$$

implies $\left\| e^{\frac{\varphi}{h}} f_h \right\|_{L^2} = \mathcal{O}(h^{3/2} \left|\log h\right|^3)$. Taking the real part of the Agmon estimate (A.1) with $u_1 = u_2 = u$, $v_1 = v_2 = e^{\frac{\theta}{h}} u$ and

$$\theta(x) = \int_a^x \sqrt{\tilde{\mathcal{V}}_h(t) - k^2 - h}\ dt \quad (= \varphi(x) + \mathcal{O}(h))$$

implies successively

$$\|v\|_{L^2} = \mathcal{O}(h^{1/2} \left|\log h\right|^3)$$

$$\int_a^b e^{\frac{\theta}{h}} f_h \overline{v}\ dx = \mathcal{O}(h^2 \left|\log h\right|^6)$$

$$\left\|hv'\right\|_{L^2}^2 = \mathcal{O}(h^2 \left|\log h\right|^6)$$

$$\|v\|_{L^\infty}^2 \leq C \left[\|v\|_{L^2}^2 + \|v\|_{L^2} \left\|v'\right\|_{L^2} \right] = \mathcal{O}(h^{1/2} |\log h|^6).$$

We conclude with

$$\left\| e^{\frac{\varphi}{h}} (\tilde{\psi}_h - \psi_h) \right\|_{L^\infty} = \mathcal{O}\left(\|v\|_{L^\infty} \right). \qquad \square$$

3. Comments.

a) The proof of Theorem 2.2 meets two critical limits of the WKB analysis.

- First, an higher order expansion $\psi_{app,h} = \psi_0 + h\psi_1$ has to be considered in order to estimate the error $\psi_h - \psi_0$. This is completely standard in the framework of WKB asymptotic expansions. With a $\mathcal{C}^\infty$-potential it is not necessary to count carefully the additional regularity or the additional terms in the expansion. Here the limited regularity requires a careful adaptation of the standar WKB method.
- The derivation of estimates with exponential weights can be viewed as a microhyperbolic propagation of regularity result with a forth and back process (see [5][4]), which is typical of a boundary value problem rather than a Cauchy problem. Here one starts from the point $x = a$ but the boundary condition at $x = b$ has to be taken into account carefully although it is only at this point that the exponentially increasing mode is comparable to the exponentially decreasing one. Here again the limited regularity and

the possibility of an asymptotically accumulated mass at $x = b$ for the h-dependent measure $\tilde{\mathcal{V}}_h''$ requires some care. It is solved by the truncation of $\tilde{\mathcal{V}}_h''$ within some intermediate scale and the accurate comparison of r_0 and r_{0h} done in the last step.

For these reasons, although it is a very simple geometric setting this problem provides a stimulating example of application of Carleman's method in WKB analysis. It is a question whether the final result can be achieved with a simpler method, without the introduction of the term $h\psi_1$ or with a less regular potential.

b) It is possible to consider this $1D$ boundary value problem with a shooting method. It is not clear that such an accurate comparison with the WKB approximation can be obtained in this way.

c) A multidimensional extension of this simple result may be interesting, with possible of applications to the modelling of nonlinear effects in quantum wires or quantum dots. The first problem is the determination of the Agmon distance as a solution to the Hamilton-Jacobi equation. With a weakly regular potential it can be naturally introduced as a viscosity solution (see [9]) but additional regularity assumptions may be necessary in order to ensure the well-posedness of the transport equations used in the WKB method. Another approach consists in considering a classical solution to the Hamilton-Jacobi equations under the assumption that the whole second derivative $(\partial_{x_i x_j}\tilde{\mathcal{V}}_h)$ is a uniformly bounded L^1-function. With this slightly stronger assumption, the Hamiltonian vector field $\xi.\partial_x + \partial_x\tilde{\mathcal{V}}_h(x)\partial_\xi$ is a divergence free $W^{1,1}$ vector field which admits unique trajectories for almost all initial data (see [8]). More safely than a BV assumption (see [7] for a brief overview and complete references), this would ensure the existence of standard (non viscosity) solutions for the Hamilton-Jacobi equation $-|\nabla\varphi|^2 + \tilde{\mathcal{V}}_h(x) = k^2$. This regularity provides also enough regularity in order to solve the transport equations of the WKB method with classical solutions. In the application of Carleman's method a conormality assumption of the singularities near the boundary may be necessary.

A. Agmon energy identity. Here we just give the basic energy identity.

Lemma A.1. *Let $\Omega := (\alpha, \beta)$ be an open interval, $V \in L^\infty(\Omega)$, $z \in \mathbb{C}$ and θ a Lipschitz real function on Ω. Denote by P the Schrödinger operator $P := -h^2 d^2/dx^2 + V$. Then for any u_1, u_2 in $H^1(\Omega)$ such that u_1'' is a bounded* *measure in* $\overline{\Omega}$*, the identity*

$$\begin{aligned}\int_\alpha^\beta e^{2\frac{\theta}{h}}(P-z)u_1\bar{u}_2dx &= \int_\alpha^\beta hv_1'\overline{hv_2'}dx + \int_\alpha^\beta (V-z-\theta'^2)v_1\bar{v}_2dx \\ &\quad + \int_\alpha^\beta h\theta'(v_1'\bar{v}_2 - v_1\bar{v}_2')dx \\ &\quad + h^2\left(e^{2\frac{\theta(\alpha)}{h}}u_1'\bar{u}_2(\alpha) - e^{2\frac{\theta(\beta)}{h}}u_1'\bar{u}_2(\beta)\right)\end{aligned} \tag{A.1}$$

holds by setting $v_j := e^{\theta/h}u_j$ *for* $j = 1, 2$*. Moreover this identity makes sense by considering the interior integral* $\int_{\alpha+0}^{\beta-0}$ *or the exterior integral* $\int_{\alpha-0}^{\beta+0}$ *while adapting the boundary terms* $u_1'(\alpha \pm 0)$ *and* $u_1'(\beta \mp 0)$*.*

This identity is obtained after conjugation of hd/dx by $e^{\theta/h}$ and integration by parts.

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IRMAR, UMR-CNRS 6625
Université Rennes 1
Campus de Beaulieu
35042 Rennes Cedex, France
e-mail: `Francis.Nier@univ-rennes1.fr`

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