Breit-Wigner formula at barrier tops

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–Dedicated to Professor N. Shimakura on the occasion of his 60th birthday–

Abstract

For non-critical energies, the asymptotic behaviour of the scattering phase and of the time-delay are known to be described by a Weyl type formula and the Breit-Wigner formula respectively. We consider here the case of critical energy levels in dimension 1. We obtain the semiclassical asymptotics of the scattering phase and of the time-delay, uniformly with respect to the energy in a neighborhood of a critical value.

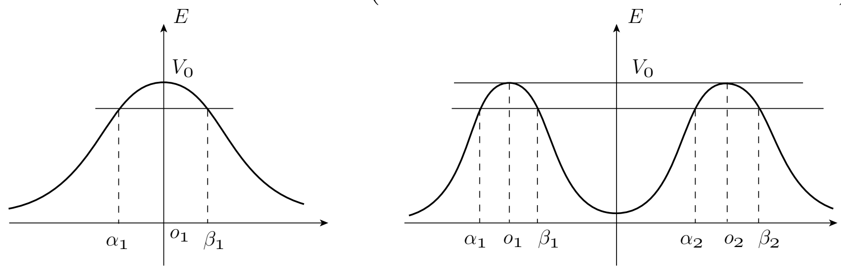
Key words: Spectral Shift Function, Scattering phase, Time-delay, Critical energy levels, Breit-Wigner formula, Schrödinger equation, Semiclassical asymptotics.

1 Introduction

We study the asymptotic behavior in the semiclassical limit of the scattering phase and the time delay for the one-dimensional Schrödinger operator

$$P(x, hD) = h^2D^2 + V(x), \quad D = \frac{1}{i}\frac{\partial}{\partial x} \tag{1}$$

for energies close to a critical value V_0 of the potential $V(x)$. We will focus here on the case where V_0 is a non-degenerate, global maximum of the potential. We shall consider the two cases where $V(x)$ reaches its maximum at one point (case I) and at two points (case II). In case I, the underlying classical system presents a saddle point, whereas in case II it presents a heteroclinic orbit between the two saddle points associated to the points of maximum. The case where V_0 is a local maximum, more precisely the case of a homoclinic orbit for the associated hamiltonian system, can be treated in the same way, and we provide also results in that case (cf. the discussion after Theorem 2.2).



case I

case II

The scattering phase $\theta(E,h)$ is a priori a very simple object, namely the argument (up to normalization, see (30) below) of the determinant of the scattering matrix (which is unitary) associated to P. The remarkable fact, proved by Birman and Krein (cf. [Bi-Kr]), is that, under suitable assumptions on the potential V, in particular when $V \to 0$ when $x \to \infty$ fastly enough, this quantity is strongly related to spectral properties of P. Indeed we have, for $E > 0$

$$\theta(E,h) = \pi s(E,h) \mod \pi\mathbb{Z}, \tag{2}$$

where $s(E,h)$ is the Spectral Shift Function (for short SSF), defined as a distribution in $\mathcal{S}'(\mathbb{R})$ by $s(E,h) = 0$ for $E << 0$, and

$$\langle s', f\rangle = \mathrm{Tr}(f(P(x,hD)) - f(h^2D^2)). \tag{3}$$

The SSF can be seen as an extension to the continuous spectrum of the counting function for the eigenvalues of P since, as one can see easily, for $E < 0$,

$$\mathcal{N}(E,h) = s(E,h), \tag{4}$$

where $\mathcal{N}(E,h)$ is the number of eigenvalues of $P(x,hD)$ not exceeding E.

As for the counting function $\mathcal{N}(E,h)$, the asymptotic behaviour of $s(E,h)$ as $h \to 0$ has been shown to be of Weylian type, but only in certain particular circumstances. Let us be more precise. We denote by $s^{\mathrm{cl}}(E)$ the classical analogue of the spectral shift function defined by

$$\langle s^{\mathrm{cl}}(E), f'(E)\rangle = -\int\int_{\mathbb{R}^{2n}} \{f(p(x,\xi)) - f(p_0(\xi))\}dxd\xi, \tag{5}$$

where $p(x,\xi) = \xi^2 + V(x)$ and $p_0(\xi) = \xi^2$ are the semiclassical symbols of P and h^2D^2 respectively. Notice that

$$s^{\mathrm{cl}}(E) = \tau_n \int_{\mathbb{R}^n} \{(E - V(x))_+^{n/2} - E_+^{n/2}\}dx, \tag{6}$$

where $a_+ = \max(a, 0)$ and τ_n is the volume of the unit sphere in $\mathbb{R}^n$. We recall also that an energy level E is said to be *non-trapping* for P if every trajectory of the Hamiltonian field H_p on $p^{-1}(E)$ escapes to infinity as time goes to both $+\infty$ and $-\infty$. D.Robert and H.Tamura (see [Ro-Ta]) have proved the following

Theorem 1.1 *If each $E \in [E_1, E_2] \subset \mathbb{R}^+$ is non-trapping, then $s(E, h)$ has a complete asymptotic expansion as $h \to 0$, uniform with respect to E in $[E_1, E_2]$. Moreover, at leading order we have*

$$s(E, h) = (2\pi h)^{-n} s^{\mathrm{cl}}(E) + O(h^{1-n}) \quad \text{as} \quad h \to 0. \tag{7}$$

When the energy is trapping, however, it is believed that the scattering phase varies very rapidly because of the presence of poles of the scattering matrix called *resonances* close to the real axis.

The case of trapping energies which are regular values of p has already been investigated, and we would like to mention here two works on the scattering phase in such a situation. In [Gé-Ma-Ro], C.Gérard, A.Martinez and D.Robert have studied the scattering phase in the presence of shape resonances (cf. [He-Sj 1]), that is resonances generated by the presence of a well in an island, which are known to be exponentially (with respect to h) close to the real axis. They have proved that the scattering phase increases by π at the real part of such a resonance. More precisely they obtain the so-called Breit-Wigner formula for the time-delay (the derivative of the scattering phase with respect to the energy). In the same situation, S.Nakamura [Na] associates to P two Hamiltonians P_{int} and P_{ext}, corresponding to the bounded and unbounded component of $p^{-1}(E)$ respectively. He shows that if E is non-trapping in some interval for P_{ext}, the spectral shift function for P is approximated in that energy interval by the sum of the SSF for P_{ext}, the asymptotic behavior of which we know from Theorem 1.1, and the eigenvalue counting function for P_{int}. These eigenvalues are close to the shape resonances of P, and cause again rapid variations of the scattering phase.

As we have already said, our concern here is the behaviour of the Spectral Shift Function for energies close to a critical value of the symbol p. We work here in the case of dimension 1, and the methods we use are not easily adaptable to higher dimensional situations (see [Br-Pe] for recent results concerning the Breit-Wigner formula in the n-dimensional, non-critical case). But we provide very precise results, which we think to be of interest for the understanding of the scattering phase in a general setting. In particular in our case II, the underlying mechanical system, though it is not chaotic, is highly unstable, and it is an important question to understand scattering data in such a situation.

In our settings, the barrier top energy $E = V_0$ is trapping since it takes infinite time for classical particles to arrive at a barrier top: it generates hyperbolic fixed points for the associated hamiltonian flow. Notice also that in case I, $E \neq V_0$ is always non-trapping, but in case II, E is non-trapping above V_0 and trapping below V_0 because of the presence of potential well.

Roughly speaking, we prove here that Robert and Tamura's formula (7) still holds in our case I, provided we replace $s^{\rm cl}(E)$ by $\sigma_{\rm ext}(E,h)$, the real part of a natural regularized classical action $s^{\rm reg}(E,h)$ (see (13) for the precise definition). Indeed $s^{\rm cl}(E)$ presents a logarithmic singularity at $E=V_0$ (see Lemma 4.1), but from our computation emerges a purely quantum contribution, closely related to the tunneling phenomenon through the barrier, which cancels the singularity. In case II, the same phenomenon takes place, and we recover Nakamura's result replacing $s^{\rm cl}(E)$ by its regularization. More precisely, $s^{\rm cl}(E)$ is then the sum of two actions $s^{\rm cl}_{\rm ext}(E)$ and $s^{\rm cl}_{\rm int}(E)$ associated to the sea and the well respectively, and these have to be replaced by $\sigma_{\rm ext}(E,h)$ and $\sigma_{\rm int}(E,h)$ respectively, the real part of the corresponding contributions in $s^{\rm reg}(E,h)$ (Theorem 2.1). Moreover, we are able to describe precisely the behaviour of $s^{\rm reg}(E,h)$ in both cases I and II in a whole interval $]V_0-\delta, V_0+\delta[$. In case II, and when $E<V_0$, we recover the Breit-Wigner formula for the time-delay. Therefore we have extended the Breit-Wigner formula to a whole neighbourhood of V_0 (Theorem 2.2).

Our starting point in this short paper is the asymptotic formulas for the scattering matrix obtained in [Ra] for the case I and in [Fu-Ra 1] for the case II. These formulas were obtained using the so-called *exact WKB analysis* (see [Gé-Gr]), together with microlocal connection formulas obtained through a reduction to a normal form (see [He-Sj 2]). In Section 1 we state our precise results. We recall shortly in Section 2 the basic facts in 1-dimensional scattering, and we present the results of [Fu-Ra 1]. We prove our results in Section 3.

2 Preliminaries and Results

We consider the one-dimensional Schrödinger equation (1) where the potential V satisfies the following assumptions:

(H1) The function V is real on $\mathbb{R}$ and dilation analytic, that is, V is holomorphic in a sector $\mathcal{S}=\{x\in\mathbb{C}; |\operatorname{Im} x|<\tan\theta_0|\operatorname{Re} x|\}\cup\{|\operatorname{Im} x|<\delta\}$ for some $0<\theta_0<\pi/2$ and $\delta>0$.

(H2) The potential V is short range, that is, there exist positive constants ϵ and C such that $|V(x)|\leq C(1+|x|)^{-1-\epsilon}$ in $\mathcal{S}$.

Let V_0 be the maximum of the potential on the real axis which we assume to be positive. We consider the two cases:

(Case I) $V^{-1}(V_0) = \{o_1\}$

(Case II) $V^{-1}(V_0) = \{o_1, o_2\} \quad (o_1 < o_2)$

From now on, we will use the convention that $*$ stands for 1 in case I and 2 in case II.

In both cases, we assume furthermore that the curvature does not vanish at each critical point:

(H3) $V''(o_j) = -\frac{1}{2\rho_j^2} < 0,\ \rho_j > 0, \quad j = 1, *.$

If $E < V_0$ and is sufficiently close to V_0, say $|E - V_0| < \delta$, the equation $V(x) - E = 0$ has 2 real roots $\alpha_1(E), \beta_1(E)$ near o_1 ($\alpha_1 < o_1 < \beta_1$) in both cases and 2 other real roots $\alpha_2(E), \beta_2(E)$ near o_2 ($\alpha_2 < o_2 < \beta_2$) in case II. We then define the action integrals between these turning points and $\pm\infty$ as follows:

$$s_j(E) = 2\int_{\alpha_j(E)}^{\beta_j(E)} \sqrt{V(x) - E}\,dx, \quad j = 1, *, \tag{8}$$

$$s_{\text{ext}}^{\text{cl}}(E) = 2\left(\int_{-\infty}^{\alpha_1(E)} + \int_{\beta_*(E)}^{\infty}\right)\{\sqrt{E - V(x)} - \sqrt{E}\}dx - 2\sqrt{E}(\beta_*(E) - \alpha_1(E)), \tag{9}$$

$$s_{\text{int}}^{\text{cl}}(E) = 2\int_{\beta_1(E)}^{\alpha_2(E)} \sqrt{E - V(x)}\,dx \quad \text{(in case II)}. \tag{10}$$

Let us remark here that the classical counterpart of the spectral shift function $s^{\text{cl}}(E)$ (see (5)) is related with these actions by

$$s^{\text{cl}}(E) = \begin{cases} s_{\text{ext}}^{\text{cl}}(E) & \text{(case I)} \\ s_{\text{ext}}^{\text{cl}}(E) + s_{\text{int}}^{\text{cl}}(E) & \text{(case II)} \end{cases} \tag{11}$$

In our results will also appear the Jost function N of the harmonic oscillator (see Remark 4.3). It is the analytic function in $\{z \in \mathbb{C}\backslash\{0\}; |\arg z| < \pi\}$ defined by

$$N(z) = \frac{\sqrt{2\pi}}{\Gamma(z + 1/2)} e^{z\log(z/e)}. \tag{12}$$

Instead of the classical actions given by (8), (9) and (10), the relevant quantities are going to be the *regularized* actions $s_{\text{ext}}^{\text{reg}}(E, h)$ and $s_{\text{int}}^{\text{reg}}(E, h)$, defined for $E < V_0$ and $|E - V_0| < \delta$ by

$$s_{\text{ext,int}}^{\text{reg}}(E, h) = s_{\text{ext,int}}^{\text{cl}}(E) + ih\log\{N(i\frac{s_1(E)}{2\pi h})N(i\frac{s_*(E)}{2\pi h})\}, \tag{13}$$

or their real parts

$$\sigma_{\rm ext,int}(E,h)=s^{\rm cl}_{\rm ext,int}(E)-h\left\{\arg N(i\frac{s_1(E)}{2\pi h})+\arg N(i\frac{s_*(E)}{2\pi h})\right\}, \tag{14}$$

where $\arg(is_j(E)/(2\pi h))=\pi/2$ for $E<V_0$. We will see in Proposition 4.4, that these functions $\sigma_{\rm ext,int}(E,h)$ can be extended as holomorphic functions of E to a whole complex neighborhood of $E=V_0$, of course depending on h. It is also important to notice already that, far from the barrier top, the functions $\sigma_{\rm ext,int}(E,h)$ coincide with $s^{\rm cl}_{\rm ext,int}(E)$ (see (43)). More precisely, in the region $|\arg\frac{is_j(E)}{2\pi h}|<\pi$, we have

$$\sigma_{\rm ext,int}(E,h)\to s^{\rm cl}_{\rm ext,int}(E)\quad\text{as}\quad |E-V_0|/h\to+\infty \tag{15}$$

At last, we will need in case II another function γ, which gives the width of the resonances: again for $E<V_0$ and $|E-V_0|<\delta$, we put

$$\gamma(E,h)=\frac{|N(i\frac{s_1(E)}{2\pi h})N(i\frac{s_2(E)}{2\pi h})|-1}{|N(i\frac{s_1(E)}{2\pi h})N(i\frac{s_2(E)}{2\pi h})|+1}. \tag{16}$$

We will also show in Lemma 4.5 that this function γ extends holomorphicaly to a complex neighborhood of $E=V_0$.

We are now able to state our results. Let us first describe the asymptotic behaviour of the scattering phase.

Theorem 2.1 *There exists $C>0$ such that if E is real and $|E-V_0|\le Ch$, then we have in case I*

$$\theta(E,h)=\frac{\sigma_{\rm ext}(E,h)}{2h}+O(h\log(1/h)), \tag{17}$$

and in case II

$$\theta(E,h)=\frac{\sigma_{\rm ext}(E,h)}{2h}+\tan^{-1}\left\{\gamma(E,h)\tan\frac{\sigma_{\rm int}(E,h)}{2h}\right\}+O(h\log(1/h)). \tag{18}$$

The asymptotic formula (17) and (18) are analoguous to the results of [Ro-Ta] and [Na] respectively. The second term in the right hand side of (18) is related to the presence of the potential well and causes rapid variations. It will be seen more clearly in the next result, describing the asymptotic behaviour of the *time delay*, which is the derivative of the scattering phase with respect to the energy E.

Theorem 2.2 *There exists $C>0$ such that if E is real and $|V_0-E|\le Ch$, then we have in case I*

$$\frac{d\theta}{dE}=\frac{\rho_1}{h}\log\frac{1}{h}+O(\frac{1}{h}). \tag{19}$$

In case II, if E is real and $|V_0 - E| \leq Ch/\log(1/h)$, then we have

$$\frac{d\theta}{dE} = \frac{\rho_1 + \rho_2}{2h} \left\{ 1 + \frac{\gamma}{(1-\gamma^2)\cos^2(\sigma_{\mathrm{int}}/2h) + \gamma^2} \right\} \log \frac{1}{h} + O(\frac{1}{h}). \tag{20}$$

We have proved a similar formula in the homoclinic case (see the end of Section 2). For example suppose V has exactly two local maxima at o_1 and o_2, with $V(o_1) < V(o_2)$. For energies E close to $V_0 = V(o_1)$, and assuming that the turning points α_2 and β_2 are simple, the formula (18) still holds, but with γ defined as

$$\gamma(E,h) = \frac{|N(i\frac{s_1(E)}{2\pi h})| - 1}{|N(i\frac{s_1(E)}{2\pi h})| + 1}. \tag{21}$$

Notice that this new definition for γ is what could be expected in view of (43). For the time delay we obtain, with this new γ,

$$\frac{d\theta}{dE} = \frac{\rho_1}{2h} \left\{ 1 + \frac{\gamma}{(1-\gamma^2)\cos^2(\sigma_{\mathrm{int}}/2h) + \gamma^2} \right\} \log \frac{1}{h} + O(\frac{1}{h}). \tag{22}$$

The reader may notice that, in each of these cases, the leading term is logarithmic with respect to h, hence one gets a non-Weylian asymptotic in these small neighborhoods of the potential maximum.

Let us add some comments about our Formula (20), in particular on the function

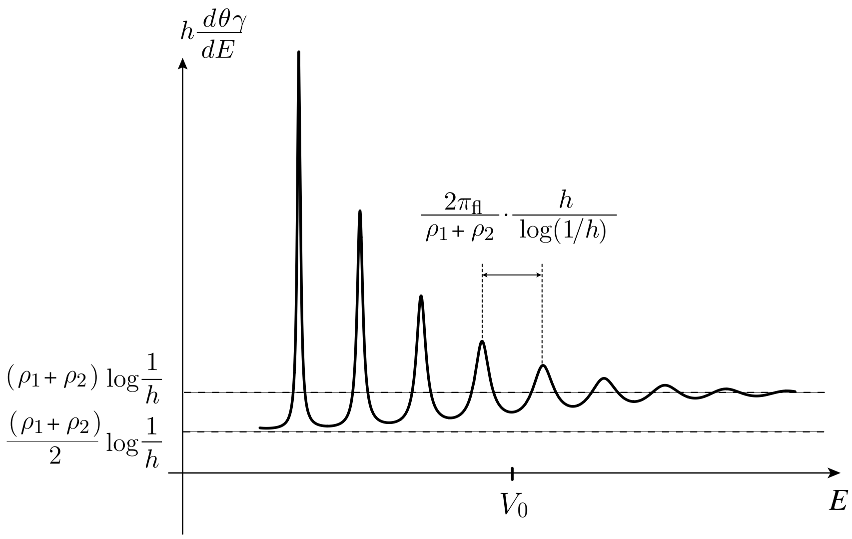
$$B(E,h) = \frac{\gamma}{(1-\gamma^2)\cos^2(\sigma_{\mathrm{int}}/2h) + \gamma^2} \tag{23}$$

which is the contribution from the potential well. As $h \to 0$, the function $\gamma(E,h)$ tends to 0 for $E < V_0$ and to 1 for $E > V_0$. It also equals 1/3 for $E = V_0$. On the other hand, when γ is small, B presents a spike at each zero of $\cos(\sigma_{\mathrm{int}}/2h)$, whose height is $1/\gamma$ and width γ (see Lemma 4.5). These zeros of $\cos(\sigma_{\mathrm{int}}/2h)$ (the real part of the resonances, see [Fu-Ra 1]) are given by the Bohr-Sommerfeld type quantization condition

$$\sigma_{\mathrm{int}}(E,h) = (2n+1)\pi h, \tag{24}$$

and, it follows from Proposition 4.4 that the distance between two such successive zeros in a complex disk centered at V_0 of radius $Ch/\log(1/h)$ is $2\pi(\rho_1+\rho_2)^{-1}h/\log(1/h)$.

Thus, as can be seen on the picture below, we have obtained an extension of the *Breit-Wigner formula* to a complete real neighbourhood of the potential maximum.



3 The Scattering Matrix

We recall here the definitions of the phase shift and of the time-delay in our one-dimensional setting. Under the assumptions (H1) and (H2), and for E in $\Pi_{\theta_0} = \{E \in \mathbb{C}\backslash\{0\}; |\arg E| < 2\theta_0\}$, there exists exactly one solution $f_r^{\pm}$ and exactly one solution $f_l^{\pm}$ of (1) such that

$$\begin{aligned} f_r^{\pm}(x) &\sim e^{\pm i\sqrt{E}x/h} \quad \text{as} \quad \operatorname{Re} x \to +\infty \quad \text{in} \quad \mathcal{S}, \\ f_l^{\pm}(x) &\sim e^{\pm i\sqrt{E}x/h} \quad \text{as} \quad \operatorname{Re} x \to -\infty \quad \text{in} \quad \mathcal{S}. \end{aligned} \tag{25}$$

These solutions (usually called Jost solutions) are holomorphic in $(x, E) \in \mathcal{S} \times \Pi_{\theta_0}$, and the two pairs (f_l^+, f_l^-) and (f_r^+, f_r^-) form two basis of the space of solutions of Equation (1). These basis are related to each other by a constant matrix (the transmission matrix) $\mathbb{T}(E, h)$:

$$\begin{pmatrix} f_l^+ \\ f_l^- \end{pmatrix} = \mathbb{T}(E,h) \begin{pmatrix} f_r^+ \\ f_r^- \end{pmatrix}. \tag{26}$$

The determinant of this matrix is 1 since $[f_l^+, f_l^-] = \det \mathbb{T}\ [f_r^+, f_r^-]$, and the wronskians $[f_l^+, f_l^-]$ and $[f_r^+, f_r^-]$ are both equal to $-2i\sqrt{E}/h$.

For a complex function $(x, E, h) \mapsto f(x, E, h)$, we will denote by f^* the function given by

$$f^*(x, E, h) = \overline{f(\bar{x}, \bar{E}, h)}.$$

It is easy to see that $f_{l,r}^- = (f_{l,r}^+)^*$, so that $\mathbb{T}$ is of the form

$$\mathbb{T} = \begin{pmatrix} a & b \\ b^* & a^* \end{pmatrix}, \quad aa^* - bb^* = 1. \tag{27}$$

Since the entries a and b can be written in terms of Jost solutions:

$$a(E,h) = \frac{ih}{2\sqrt{E}}[f_l^+, f_r^-], \quad b(E,h) = -\frac{ih}{2\sqrt{E}}[f_l^+, f_r^+], \tag{28}$$

they are holomorphic in $E \in \Pi_{\theta_0}$, as well as $a^*(E,h)$ and $b^*(E,h)$.

The scattering matrix is defined as the matrix associated with the change of basis between the outgoing pair of solutions (f_r^+, f_l^-) and the incoming pair of solutions (f_l^+, f_r^-): if

$$p_+ f_r^+ + p_- f_l^- = q_+ f_l^+ + q_- f_r^-,$$

then

$$\begin{pmatrix} p_+ \\ p_- \end{pmatrix} = \mathbb{S}(E,h) \begin{pmatrix} q_+ \\ q_- \end{pmatrix}.$$

In terms of a and b we immediately have

$$\mathbb{S} = \frac{1}{a^*} \begin{pmatrix} 1 & -b^* \\ b & 1 \end{pmatrix}. \tag{29}$$

Suppose now that E is a positive real number. Then $\mathbb{S}(E,h)$ is unitary by (27), and its determinant is a complex number of modulus 1. The scattering phase $\theta(E,h)$ is defined as half of the argument of $\det \mathbb{S}$:

$$\det \mathbb{S}(E,h) = e^{2i\theta(E,h)}. \tag{30}$$

The function θ is real, and it can be written as

$$\theta(E,h) = \arg a(E,h) = -\arg a^*(E,h). \tag{31}$$

Thus, what we have to do in order to prove our Theorem 2.1, is to examine the asymptotic behaviour of $a^*(E,h)$ obtained in [Ra] and [Fu-Ra 1] (see also [Fu]).

Theorem 3.1 *There exists $h_0 > 0$ and $C > 0$ such that, for all $h \in]0, h_0]$ and all $E \in D(V_0, Ch)$, one has in case I:*

$$a^*(E,h) = e^{(s_1(E) - i s_{\text{ext}}^{\text{cl}}(E))/2h} N(i\frac{s_1(E)}{2\pi h})(1 + O(h \log h)), \tag{32}$$

whereas, in case II,

$$\begin{aligned} a^*(E,h) = {} & e^{(s_1(E)+s_2(E)-i s_{\text{ext}}^{\text{cl}}(E))/2h} \\ & \left(e^{i s_{\text{int}}^{\text{cl}}(E)/2h} + N(i\tfrac{s_1(E)}{2\pi h}) N(i\tfrac{s_2(E)}{2\pi h}) e^{-i s_{\text{int}}^{\text{cl}}(E)/2h}\right)(1 + O(h \log h)). \end{aligned} \tag{33}$$

For later needs, we notice that $\theta(E,h)$ can also be defined as a complex-valued function of complex $E \in \Pi_{\theta_0}$ by

$$\theta(E,h) = \frac{1}{2i} \log \frac{a(E,h)}{a^*(E,h)}. \tag{34}$$

Indeed, since a and a^* are holomorphic in Π_{θ_0}, $\theta(E,h)$ is singular only at zeros of a and a^*. The zeros of a are complex conjugates of those of a^*, and it is enough to study the asymptotic distribution of zeros of a^*. This was done in [Ra] and [Fu-Ra 1] in cases I and II respectively, through Theorem 3.1, using also Rouché's theorem. We obtain the following result.

Lemma 3.2 *There exists $C > 0$ such that $\theta(E,h)$ extends holomorphically to the disk $|E - V_0| < Ch$ in case I, and to the disk $|E - V_0| < Ch \log(1/h)$ in case II.*

Let us explain shortly how we obtained Theorem 3.1. We use here the notations and conventions of [Fu] (in particular for the normalization of the solutions). We compute a transition matrix at each maximum T_j, $j = 1, *$, the transition matrix T_l between $-\infty$ and α_1, and the transition matrix T_r between β_* et $+\infty$. In case II, we compute also a transition matrix T_{12} between β_1 and α_2. Then the transition matrix $\mathbb{T}$ can be written as

$$\mathbb{T} = T_l \cdot T_1 \cdot T_r, \tag{35}$$

in case I, and, in case II as

$$\mathbb{T} = T_l \cdot T_1 \cdot T_{12} \cdot T_2 \cdot T_r. \tag{36}$$

In [Fu-Ra 1] the following result is proved (see also [Fu], Proposition 3 for the definitions of the transition mastrices T_l, T_1, T_{12}, T_2, T_r and the classical actions S_l, S_r associated to $-\infty$ and $+\infty$ respectively).

Proposition 3.3 *1. There exist $R > 0$ and $\epsilon > 0$ such that*

$$T_l = \sqrt[4]{E} \begin{pmatrix} e^{i\pi/4} e^{-iS_l(E)/h}(1 + O(h)) & O(e^{-\epsilon/h}) \\ O(e^{-\epsilon/h}) & e^{-i\pi/4} e^{iS_l(E)/h}(1 + O(h)) \end{pmatrix}, \tag{37}$$

$$T_r = \frac{1}{\sqrt[4]{E}} \begin{pmatrix} e^{-i\pi/4} e^{-iS_r(E)/h}(1 + O(h)) & O(e^{-\epsilon/h}) \\ O(e^{-\epsilon/h}) & e^{i\pi/4} e^{iS_r(E)/h}(1 + O(h)) \end{pmatrix}, \tag{38}$$

$$T_{1,2} = \begin{pmatrix} e^{is_{\mathrm{int}}(E)/2h}(1 + O(h)) & O(e^{-\epsilon/h}) \\ O(e^{-\epsilon/h}) & e^{-is_{\mathrm{int}}(E)/2h}(1 + O(h)) \end{pmatrix}, \tag{39}$$

uniformly with respect to E in every compact subset of $D(V_0, R)$.

2. For any $r > 0$, one has

$$T_j = e^{s_j(E)/2h} \begin{pmatrix} N(-\frac{is_j(E)}{2\pi h})(1+O(h\log h)) & 1+O(h) \\ 1+O(h) & N(\frac{is_j(E)}{2\pi h})(1+O(h\log h)) \end{pmatrix}, \quad (40)$$

uniformly with respect to E in every compact subset of $D(V_0, rh)$.

Theorem 2.1 follows immediately from this Proposition. Notice also that we can obtain that way the scattering matrix in the homoclinic case. Then formula (36) still holds for the scattering matrix for these energies, but T_2 now reads

$$T_2 = e^{s_2(E)/2h} \begin{pmatrix} 1+O(h\log h) & 1+O(h) \\ 1+O(h) & 1+O(h\log h) \end{pmatrix}.$$

Thus, in this case, we get as in Theorem 2.1,

$$\begin{aligned} a^*(E,h) = {} & e^{(s_1(E)+s_2(E)-is^{\rm cl}_{\rm ext}(E))/2h} \\ & \left(e^{is^{\rm cl}_{\rm int}(E)/2h} + N(i\tfrac{s_1(E)}{2\pi h})e^{-is^{\rm cl}_{\rm int}(E)/2h}\right)(1+O(h\log h)). \end{aligned} \quad (41)$$

4 Proofs

We proceed first to the proof of Theorem 2.1, that is, we calculate the argument of a^* through (32) and (33). For shorter expressions, we put

$$r_j(E,h) = |N(i\frac{s_j(E)}{2\pi h})|, \quad \phi_j(E,h) = \arg N(i\frac{s_j(E)}{2\pi h}). \quad (42)$$

In case I, we get immediately

$$\theta(E,h) = \frac{s^{\rm cl}_{\rm ext}}{2h} - \phi_1 + O(h\log h) = \frac{\sigma_{\rm ext}}{2h} + O(h\log h).$$

In case II, we have

$$\begin{aligned} \theta(E,h) &= \frac{s^{\rm cl}_{\rm ext}}{2h} - \arg\left(e^{is^{\rm cl}_{\rm int}/2h} + r_1r_2e^{i(\phi_1+\phi_2)}e^{-is^{\rm cl}_{\rm int}/2h}\right) + O(h\log h) \\ &= \frac{\sigma_{\rm ext}}{2h} - \arg\left(e^{i\sigma_{\rm int}/2h} + r_1r_2e^{-i\sigma_{\rm int}/2h}\right) + O(h\log h), \end{aligned}$$

and since

$$\arg\left(e^{i\sigma_{\rm int}/2h} + r_1r_2e^{-i\sigma_{\rm int}/2h}\right) = \arg\left\{(1+r_1r_2)\cos\frac{\sigma_{\rm int}}{2h} + i(1-r_1r_2)\sin\frac{\sigma_{\rm int}}{2h}\right\}$$

$$= \tan^{-1}\left(\frac{1-r_1r_2}{1+r_1r_2}\tan\frac{\sigma_{\rm int}}{2h}\right),$$

we get (18). This ends the proof of Theorem 2.1.

In order to prove our second result, we will have to investigate some analyticity properties of terms appearing in the R.H.S. of (32) and (33). Let us begin with the action integrals $s_j(E)$, $s_{\rm ext}^{\rm cl}(E)$ and $s_{\rm int}^{\rm cl}(E)$: they were defined for $E < V_0$, $|E - V_0| < \delta$ in Section 1. See [Fu-Ra 1] for the proof of the following lemma (with slightly different notations).

Lemma 4.1 *There exist a positive constant R and functions g_j, $j = 1, 2$, $g_{\rm ext}$ and $g_{\rm int}$ holomorphic in $D(0, R)$, such that $s_j(E)$, $s_{\rm ext}^{\rm cl}(E)$ and $s_{\rm int}^{\rm cl}(E)$ are all real for $0 < V_0 - E < R$ and*

$$s_j(E) = 2\pi\rho_j(V_0 - E)(1 + (V_0 - E)g_j(V_0 - E)) \quad (j = 1, 2),$$

$$s_{\rm ext,int}^{\rm cl}(E) = s_{\rm ext,int}^{\rm cl}(V_0) + \frac{1}{2\pi}(s_1(E) + s_*(E))\log(V_0 - E) + (V_0 - E)g_{\rm ext,int}(V_0 - E).$$

where $\log\lambda > 0$ when $\arg\lambda = 0$.

We also recall some properties of the function $N(z)$.

Lemma 4.2 *$N(z)$ is holomorphic in $\{z \in \mathbb{C}\backslash\{0\}; |\arg z| < \pi\}$ and in this domain,*

$$\lim_{|z|\to\infty} N(z) = 1. \tag{43}$$

In particular, on the positive imaginary axis $z = it, t > 0$, we have

$$|N(it)|^2 = 1 + e^{-2\pi t}, \tag{44}$$

$$\arg N(it) = t\log t + tg(t), \tag{45}$$

where g is a real and analytic function and extends holomorphically to a complex neighborhood of the origin.

Proof: The formula (43) is nothing else than Stirling formula, and (44) follows easily from the product formula of the Gamma function:

$$|\Gamma(\frac{1}{2} + it)|^2 = \Gamma(\frac{1}{2} + it)\Gamma(\frac{1}{2} - it) = \frac{\pi}{\cosh\pi t}. \tag{46}$$

For (45), we have

$$\arg N(it) = t\log t - t - \arg\Gamma(1/2 + it).$$

Using (46), we can rewrite the last term of the right hand side as

$$\arg\Gamma(\frac{1}{2} + it) = \frac{i}{2}\log\pi - i\log\Gamma(\frac{1}{2} + it) - \frac{i}{2}\log(\cosh\pi t).$$

This function can be extended analytically to $\mathbb{C}\backslash i(\mathbb{Z}+1/2)$ and equals 0 when $t = 0$. Hence we can write $\arg N(it)$ in the form (45). □

Remark 4.3 *The function $N(z)$ can be characterized as the Jost function of the harmonic oscillator (see [Vo]). Let $\psi_\pm(x)$ be the solutions to (1) with $V(x) = x^2$ and $h = 1$ whose asymptotic behavior at $\pm\infty$ is given by*

$$\psi_\pm(x) \sim (x^2 - E)^{-1/4} \exp\left(\pm \int_{x_0}^{x} (y^2 - E)^{1/2} dy\right) \quad \text{as} \quad x \to \mp\infty.$$

It is possible to define these solutions for arbitrary $x_0 \in \mathbb{R}$ when E is negative. Then the Jost function of the harmonic oscillator, which is defined as the wronskian of these solutions, is independent of x_0 and given by

$$\frac{1}{2}[\psi_+, \psi_-] = N(-\frac{E}{2}).$$

The following result justifies in particular the terminology *regularized* actions.

Proposition 4.4 *There exists $C > 0$ such that the functions $\sigma_{\text{ext}}(E, h)$ and $\sigma_{\text{int}}(E, h)$ can be extended as holomorphic functions with respect to E in $D(V_0, Ch)$. Moreover the following asymptotic formula holds in this domain:*

$$\sigma_{\text{ext,int}}(E, h) = s^{\text{cl}}_{\text{ext,int}}(V_0) - (\rho_1 + \rho_*)(V_0 - E) \log \frac{1}{h} + O(V_0 - E) \quad \text{as} \quad h \to 0.$$

Proof: From Lemmas 4.1 and 4.2, we get

$$\sigma_{\text{ext,int}}(E, h) = s^{\text{cl}}_{\text{ext,int}}(V_0) - (\rho_1 + \rho_*)(V_0 - E) \log \frac{1}{h} + G(V_0 - E, h),$$

with

$$G(V_0 - E, h) = (V_0 - E) g_{\text{ext,int}}(V_0 - E) - \sum_{j=1,*} \left[\frac{s_j}{2\pi} \left\{ g(\frac{s_j}{2\pi h}) + \log\left(\rho_j(1 + (V_0 - E) g_j)\right) \right\} + \rho_j (V_0 - E)^2 g_j \log \frac{1}{h} \right].$$

□

At last, let us observe some properties of the function $\gamma(E, h)$.

Lemma 4.5 *There exist positive C and R such that the function $E \mapsto \gamma(E, h)$ is holomorphic in $(V_0 - R, V_0 + R) \times i(-Ch, Ch)$. Moreover, on $(V_0 - R, V_0 + R)$ in particular, $0 < \gamma < 1$ and*

(i) *if $\lambda = O(h)$, there exist $0 < \gamma_0 < \gamma_1 < 1$ independent of λ and of h such that $\gamma_0 < \gamma(E, h) < \gamma_1$ and in particular $\gamma(V_0, h) = 1/3$,*

(ii) *if* $|(V_0 - E)/h| \to \infty$,

$$\gamma(E,h) = \begin{cases} O(e^{-s_1(E)/h} + e^{-s_2(E)/h}) & (E < V_0), \\ 1 - O(e^{(s_1(E)+s_2(E))/2h}) & (E > V_0). \end{cases}$$

Proof: With (44), one obtains

$$\gamma(E,h) = \frac{\sqrt{1+e^{-s_1(E)/h}}\sqrt{1+e^{-s_2(E)/h}} - 1}{\sqrt{1+e^{-s_1(E)/h}}\sqrt{1+e^{-s_2(E)/h}} + 1},$$

and the lemma follows easily. In particular this function has singularities at the points satisfying $s_j(E) = (2n+1)\pi i h$ $(j = 1, 2)$. □

Now we can deduce Theorem 2.2 from Theorem 2.1, making use of the analyticity of the remainder terms. Indeed, let $R_I(E,h)$, $R_{II}(E,h)$ be the the remainder terms of (17), (18) respectively:

$$R_I(E,h) = \theta(E,h) - \frac{\sigma_{\rm ext}(E,h)}{2h},$$

$$R_{II}(E,h) = \theta(E,h) - \frac{\sigma_{\rm ext}(E,h)}{2h} - \tan^{-1}\left\{\gamma(E,h)\tan\frac{\sigma_{\rm int}(E,h)}{2h}\right\}.$$

We have the following key result.

Proposition 4.6 *There exists $C > 0$ such that $R_I(E,h)$ and $R_{II}(E,h)$ are holomorphic with respect to E in $D(V_0, Ch)$ and in $D(V_0, Ch/\log(1/h))$ respectively, for all sufficiently small h.*

Proof: The functions $\theta(E,h)$ and $\sigma_{\rm ext}(E,h)$ are holomorphic in the required domain by Lemma 3.2 and Proposition 4.4. It remains to show that the last term of R_{II} is also holomorphic in $D(V_0, Ch/\log(1/h))$. Let us calculate the derivative:

$$\left\{\tan^{-1}\left(\gamma\tan\frac{\sigma_{\rm int}}{2h}\right)\right\}' = \frac{1}{2h}\frac{\gamma\sigma'_{\rm int} + 2h\gamma'\cos(\sigma_{\rm int}/2h)\sin(\sigma_{\rm int}/2h)}{(1-\gamma^2)\cos^2(\sigma_{\rm int}/2h) + \gamma^2}. \tag{47}$$

Both γ and $\sigma_{\rm int}$ being holomorphic, it suffices to see that the denominator $d(E,h) = (1-\gamma^2)\cos^2(\sigma_{\rm int}/2h) + \gamma^2$ does not vanish in $D(V_0, Ch/\log(1/h))$. First we see that for real E in this domain, $d(E,h)$ is real and bounded from below by a positive constant independent of both E and h. Next for complex E, we see

$$\gamma(E,h) \to \frac{1}{3}, \quad |\,{\rm Im}\,\frac{\sigma_{\rm int}}{2h}| \le C(\rho_1 + \rho_2) + O\left(\frac{1}{\log(1/h)}\right),$$

as h tends to 0. Hence, by continuity, $d(E,h)$ stays away from 0 for sufficiently small C and h. □

Proposition 4.6 enables us to estimate the derivatives of R_I and R_{II} in terms of themselves by Cauchy's integral formula; if a function $R(\lambda)$ is holomorphic in $\overline{D(r)}$, then its derivative is bounded from above in $D(r/2)$ by $2\sup_{D(r)}|R(\lambda)|/r$. Recalling that $R_I = O(h\log(1/h))$ and $R_{II} = O(h\log(1/h))$, we obtain

$$\frac{dR_I}{dE} = O(\log(1/h)), \quad \frac{dR_{II}}{dE} = O((\log h)^2).$$

On the other hand, we know from Proposition 4.4 that

$$\frac{d\sigma_{\text{ext,int}}}{dE} = (\rho_1 + \rho_*)\log\frac{1}{h} + O(1)$$

and since $hd\gamma/dE = O(1)$

$$h\frac{d}{dE}\left\{\tan^{-1}\left(\gamma\tan\frac{\sigma_{\text{int}}}{2h}\right)\right\} = (\rho_1+\rho_2)\frac{\gamma}{(1-\gamma^2)\cos^2(\sigma_{\text{int}}/2h)+\gamma^2}\log\frac{1}{h} + O(1)$$

This completes the proof of Theorem 2.2.

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