Exact WKB analysis and the Langer modification with application to barrier top resonances

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1 Introduction and results

The main goal of this paper is to rigorously justify the well-known Langer modification (see [Be-Mo],[Fr-Fr] and [La 2]) in the framework of exact WKB analysis. More precisely, we want to describe the semiclassical behaviour in a neighbourhood of $x = 0$ of the solutions of the radial Schrödinger equation

$$-h^2\frac{d^2u}{dx^2} + \{V(x) + \frac{h^2\ell(\ell+1)}{x^2}\}u = Eu, \tag{1}$$

where ℓ is a fixed positive integer (the angular quantum number).

Our initial motivation was the study of the scattering matrix for this equation, for energies close to a local quadratic maximum of the potential V. In particular we wanted to obtain quantization conditions and we wil also, as an application, describe briefly our results in that direction. The proofs are to be found in [Fu-Ra 2].

Let us begin with our assumptions. Without loss of generality, we suppose from now on that $E = 0$ and that

- **(A1)** $xV(x)$ is holomorphic in a neighbourhood Ω of the origin and real-valued on the positive real axis, so that $V(x)$ has the Laurent expansion $V(x) = \dfrac{q_{-1}}{x} + q_0 + q_1 x + \cdots$ with real q_j's.

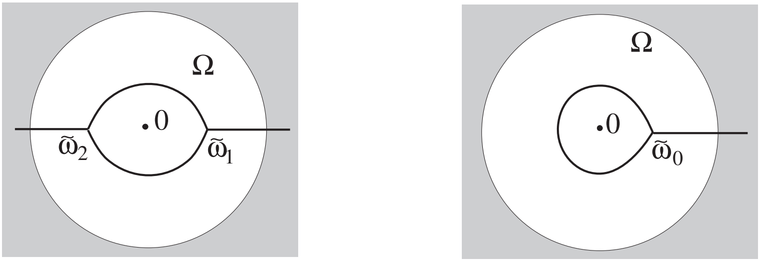
(A2) If $q_{-1} = 0$, then $q_0 \neq 0$.

Under the assumption (A1), and for fixed h, the origin is a regular singular point with exponents $\ell + 1$ and $-\ell$, and the space of solutions which goes to 0 as x does is one-dimensional. Now from the WKB point of view, we have two different cases: the case $(\mathrm{I})_\pm$ where $q_{-1} = 0$ and $\pm q_0 > 0$ and the case $(\mathrm{II})_\pm$ where $\pm q_{-1} > 0$. In case (I) the effective potential $Q(x,h) = V(x) + h^2\ell(\ell+1)/x^2$ has two simple zeros (turning points) $\omega_{1,2}(h)$ inside Ω at distance $O(h)$ from the origin, so that they coalesce with the double pole at the origin as $h \to 0$. In case (II), $Q(x,h)$ has in Ω only one simple zero $\omega_0(h)$ at distance $O(h^2)$ from the origin. Notice that in case (II) the turning point $\omega_0(h)$ is real, and so are $\omega_{1,2}(h)$ in case $(\mathrm{I})_-$. In case $(\mathrm{I})_+$, these turning points are complex conjugate, but our analysis works just as well.

In any case, the asymptotic expansion in h of a WKB solution defined near the origin is not uniform with respect to x when x tends to the origin because of the double pole of the centrifugal potential $h^2\ell(\ell+1)/x^2$. In fact, since this term dominates at the origin, the leading term $Q^{-1/4}\exp\{\pm\int^x Q^{1/2}dx'/h\}$ of a WKB solution would be equivalent neither to $x^{\ell+1}$ nor to $x^{-\ell}$ but to $x^{1/2\pm\sqrt{\ell(\ell+1)}}$. The usual way physicists handle the problem is to replace $\ell(\ell+1)$ by $(\ell+1/2)^2$ and to use Airy type connection formulas at the turning point with no further justification. In order to clear up the problem, Langer has proposed to change variables so that the singularity at the origin maps away to $-\infty$ (see [La 2]),

$$\begin{cases} x = e^y, \\ x^{-1/2}u(x) = w(y). \end{cases} \tag{2}$$

Our aim here is to justify this approach rigorously and to give precise estimates for the resulting connection formulas.



I: $\tilde\omega_{1,2}(h)=O(h)$

II: $\tilde\omega_0(h)=O(h^2)$

Figure 1: Stokes lines near the origin.

Let $\tilde{Q}(x,h)$ be the modified effective potential $\tilde{Q}(x,h) = V(x) + h^2(\ell+1/2)^2/x^2$ and $\tilde{\omega}_{1,2}$, $\tilde{\omega}_0$ the corresponding turning points. We have sketched in Figure 1 the Stokes lines emanating from the turning points, defined as the set of $x \in \Omega$ such that

$$\mathrm{Re} \int_{\tilde{\omega}}^{x} \tilde{Q}(t,h)^{1/2} dt = 0,$$

where $\tilde{\omega}$ is one of $\tilde{\omega}_{1,2}$ and $\tilde{\omega}_0$ depending on the case (I)$_\pm$ and (II). Notice that we follow here the definition in [Ge-Gr] for example, but the Stokes lines are often defined as lines where the imaginary part of the above integral vanishes. The figures are symmetric with respect to the real axis since V is real on $\mathbb{R}$. We also use the fact that ℓ is positive, so that the Stokes lines near the origin are closed curves.

We have first the following theorem, which shows in particular that the solutions which vanish at the origin can be written in a WKB form: (see also [La 1] and [Ol] where the solutions are described in terms of the solutions of a related Bessel equation.)

Theorem 1 *Let $u^0(x,h)$ be a solution of (1) which goes to 0 as x does for any small enough fixed $h > 0$ and let $\tilde{\omega}$ be one of the turning points $\tilde{\omega}_1$ and $\tilde{\omega}_2$ in case (I) and $\tilde{\omega}_0$ in case (II). Then we have for sufficiently small $x \in \Omega$ and up to a multiplicative constant,*

$$u^0(x,h) = \frac{1}{\tilde{Q}^{1/4}} \exp\left(\frac{1}{h}\int_{\tilde{\omega}}^{x} \tilde{Q}^{1/2} dx\right)(1 + a(x,h))$$

with the following estimates on the error term $a(x,h)$:

$$a(x,h) = \begin{cases} O(\frac{x^2}{h^2}) & \text{as } \frac{x}{h} \to 0 \quad \text{in case (I)}, \\ O(\frac{x}{h^2}) & \text{as } \frac{x}{h^2} \to 0 \quad \text{in case (II)}. \end{cases}$$

For the calculation of the scattering matrix for example, we need the asymptotic expansion of u^0 on the positive real axis sufficiently far from the origin. Let $I = [\epsilon, \epsilon'] \subset \Omega$ be an interval of the real axis, with $0 < \epsilon < \epsilon'$ independent of h. We may suppose I contains no zero of $\tilde{Q}$ for any h small enough. On this interval, $\pm\tilde{Q} > 0$ in cases (I)$_\pm$ and (II)$_\pm$, and

Theorem 2 *We have for $x \in I$ and up to a multiplicative constant,*

$$u^0(x,h) = \frac{1}{\sqrt[4]{\tilde{Q}}} \exp\left(\frac{1}{h}\int_{x_0}^{x} \sqrt{\tilde{Q}} dx\right)(1 + b(x,h)) \tag{3}$$

in cases (I)$_+$ and (II)$_+$, and

$$u^0(x,h) = \frac{1}{\sqrt[4]{-\tilde{Q}}} \sin(\frac{1}{h}\int_{\tilde{\omega}}^{x} \sqrt{-\tilde{Q}}dx + \frac{\pi}{4})(1+c(x,h)) \qquad (4)$$

in cases (I)$_-$ and (II)$_-$, where x_0 is an arbitrary point in I and the error terms $b(x,h)$ and $c(x,h)$ are of $o(1)$ as h tends to 0 uniformly for $x \in I$.

Remark 3 *The choice of $x_0 \in I$ in (3) does not matter since it only amounts to multiplication by a constant.*

The action integral $\int_{\tilde{\omega}}^{x} \sqrt{-\tilde{Q}}dx$ in (4) of Theorem 2 can be written in terms of the physical potential $V(x)$. Indeed it is holomorphic with respect to h in case (II)$_-$. This is also true in case (I)$_-$ under the further assumption:

(A3) In case (I)$_-$, $V(x)$ is an even function.

We can then calculate the first two terms of the Taylor expansion of the action integral (see Section 4) and get a more transparent form of (4):

Corollary 4 *Suppose the assumptions (A1–3) hold. Let $c(x,h)$ be the functions defined in Theorem 2. Then we have, still for $x \in I$ and up to a multiplicative constant,*

$$u^0(x,h) = \frac{1}{\sqrt[4]{-V}} \sin(\frac{1}{h}\int_{0}^{x} \sqrt{-V}dx - \delta)(1+c(x,h)),$$

where

$$\delta = \begin{cases} \ell\pi/2 & \text{in case (I)}_-, \\ (\ell+1/4)\pi & \text{in case (II)}_-. \end{cases}$$

Remark 5 *In case where V is a non-zero constant, the solution u^0 is a Bessel function, and we get the same formula as in Theorem 2 from its asymptotic expansion at $+\infty$. The case (II) with $V(x) = q_{-1}/x$ was studied in [La 2].*

The plan of the paper is the following: Section 1 is this introduction. In Section 2 we recall the exact WKB method along the line of [Ge-Gr] in the simple setting where the potential is independent of h. Section 3 is devoted to the proof of Theorems 1 and 2. In Section 4 we prove

Corollary 4 through a complete study of the action integrals associated with $\tilde{Q}$. As an application, we present in Section 5 our results on the scattering matrix in case where the potential V presents a quadratic barrier. We also give a quantization rule for the resonances close to the critical energy level.

2 The exact WKB method

In this section we recall briefly the exact WKB method along the line of [Ge-Gr]. This formulation of the WKB method owes much to J.Ecalle and A.Voros ([Ec], [Vo]). Of course it is very close to what the reader can find in the book [Ol]. We write the Schrödinger equation (1) as

$$\{-h^2\frac{d^2}{dx^2}+Q(x)\}u=0, \tag{5}$$

and we assume here for simplicity that Q is independent of h. We work here in a quite formal way, but the arguments can be justified in many situations, as for example at the end of this section or in Section 3 below.

First we change the independent variable by $x \mapsto z=\int_{x_0}^{x} Q(x')^{1/2}dx'$ and we get

$$(-h^2\frac{d^2}{dz^2}+2h^2H(z)\frac{d}{dz}+1)u=0,$$

where $2H(z(x)) = d(Q(x)^{-1/2})/dx$. Then we change the dependent variable:

$$u=\exp\{\int^z H(z')dz' \pm z/h\}W(z)=Q(x)^{-1/4}e^{\pm z(x)/h}W(z(x))$$

and we obtain

$$\{-\frac{d}{dz}(\frac{d}{dz}\pm\frac{2}{h})+H^2-H'\}W=0, \tag{6}$$

where $'$ stands for the differentiation with respect to z. The solution of the equation (6) can be constructed by solving inductively the following first order differential equations:

$$\begin{cases} W_0^{\pm} &= 1, \\ (\frac{d}{dz}\pm\frac{2}{h})W_{2p+1}^{\pm} &= -H(z)W_{2p}^{\pm} \quad (p\geq 0), \\ \frac{d}{dz}W_{2p}^{\pm} &= -H(z)W_{2p-1}^{\pm} \quad (p\geq 1). \end{cases} \tag{7}$$

This recurrence equations can be written in integral form if we impose initial conditions $W_n^{\pm}|_{z=z_1} = 0$ $(n \geq 1)$ for a base point $z_1 = z(x_1)$ where x_1 is not a zero of $Q(x)$:

$$\left\{ \begin{array}{ll} W_0^{\pm} & = 1, \\ W_{2p+1}^{\pm} & = -I_{\pm}[W_{2p}^{\pm}] \quad (p \geq 0), \\ W_{2p}^{\pm} & = -J[W_{2p-1}^{\pm}] \quad (p \geq 1), \end{array} \right. \tag{8}$$

where

$$I_{\pm}[f] = \int_{z_1}^{z} e^{\pm 2(t-z)/h} H(t) f(t) dt, \quad J[f] = \int_{z_1}^{z} H(t) f(t) dt. \tag{9}$$

We write

$$W^{\pm}(z; z_1, h) = W_{\text{even}}^{\pm}(z; z_1, h) + W_{\text{odd}}^{\pm}(z; z_1, h), \tag{10}$$

$$W_{\text{even}}^{\pm} = \sum_{p=0}^{\infty} W_{2p}^{\pm}(z; z_1, h), \quad W_{\text{odd}}^{\pm} = \sum_{p=0}^{\infty} W_{2p+1}^{\pm}(z; z_1, h), \tag{11}$$

and the main feature of this construction is that the series (11) are convergent and give also asymptotic expansions in certain domains. More precisely, we have the following:

Proposition 6 *Let D be a domain in the z-plane where $Q(x(z))$ is holomorphic and does not vanish. Suppose $z_1 \in D$ and let $D_{\pm}$ be the set of z in D such that there exists a path from z_1 to z along which $\pm \operatorname{Re} z$ is strictly increasing. Then the two series in (11) converge absolutely in a neighborhood of z_1 and extend holomorphically to D. Moreover, we have for all $N \in \mathbb{N}$,*

$$\begin{array}{l} W_{\text{even}}^{\pm}(z; z_1, h) - \sum_{p=0}^{N} W_{2p}^{\pm}(z; z_1, h) = O(h^{N+1}) \quad \text{in} \quad D_{\pm}, \\ W_{\text{odd}}^{\pm}(z; z_1, h) - \sum_{p=0}^{N} W_{2p+1}^{\pm}(z; z_1, h) = O(h^{N+1}) \quad \text{in} \quad D_{\pm}. \end{array} \tag{12}$$

Returning to the x-variable, we denote the solutions of the equation (5) constructed as above by

$$w_{\pm}(x, h; x_0, x_1) = Q(x)^{-1/4} e^{\pm z(x)/h} W^{\pm}(z(x); z(x_1), h).$$

By Proposition 6, these solutions are exact and have the WKB asymptotic expansion in $z^{-1}(D_{\pm})$. We call them *exact WKB solutions.*

In order to obtain connection formulas, we need at last to compute the Wronskian of two exact WKB solutions. Setting

$$w_j^{\pm} = w_{\pm}(x, h; x_0, x_j) = Q(x)^{-1/4} e^{\pm z(x)/h} W^{j,\pm}(z(x)), \quad (j = 1, 2),$$

and denoting by $[w_1^+, w_2^-]_x = w_1^+(w_2^-)' - (w_1^+)'w_2^-$ their Wronskian, we see that

$$\begin{aligned}[w_1^+, w_2^-]_x &= [e^{z/h}W^+(z;z_1), e^{-z/h}W^-(z;z_2)]_z \\ &= [W^+(z;z_1), W^-(z;z_2)]_z - \frac{2}{h}W^+(z;z_1)W^-(z;z_2).\end{aligned}$$

We use the recurrence equations (7) to compute the Wronskian with respect to z, and then substitute $z = z_2 = z(x_2)$ since the Wronskian is independent of the variable. We have $W^-_{\mathrm{even}}(z_2;z_2) = 1$, $W^-_{\mathrm{odd}}(z_2;z_2) = 0$ and we get

Proposition 7 *Let $w_j^\pm$ be the exact WKB solutions defined as above and $z = \int_{x_0}^{x_2} Q^{1/2}dx$. Then*

$$[w_1^+, w_2^-]_x = -\frac{2}{h}W^+_{\mathrm{even}}(z_2;z_1,h). \tag{13}$$

Finally we show, as an example, how the exact WKB method yields local connection formulas near a simple turning point. We suppose here that $Q(x)$ is real on $\mathbb{R}$ and holomorphic near some $\alpha \in \mathbb{R}$ where $Q(\alpha) = 0$, $Q'(\alpha) > 0$. Such an α is called a simple turning point for the equation (5). Recalling that the Stokes lines are the level curves of the function $\mathrm{Re}z(x)$ with $z(x) = \int_\alpha^x Q^{1/2}dx$, it is easily seen that three Stokes lines start from such a simple turning point (see Figure 2).

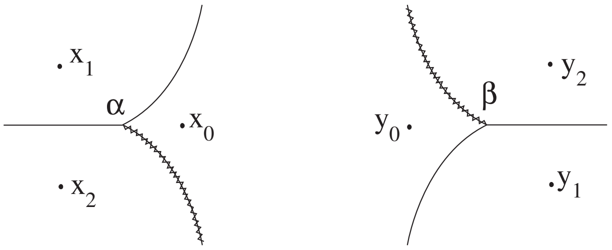


Figure 2: Stokes lines near simple turning points.

Now we suppose that $Q^{1/2}$ is positive for $x > \alpha$ and we fix the determination of $Q^{1/2}$ by drawing a cut as in Figure 2. The wiggly lines in the figure stand for the branch cuts. We also choose some base points x_j, $j = 0, 1, 2$ as in Figure 2 and we define three exact WKB solutions:

$$\begin{aligned}U_0 &= e^{\pi i/4}w_-(x,h;\alpha,x_0),\\ U_1 &= e^{-\pi i/4}w_+(x,h;\alpha,x_1),\\ U_2 &= e^{\pi i/4}w_-(x,h;\alpha,x_2).\end{aligned}$$

It is important here to notice that we have chosen these solutions so that the asymptotic expansions (12) are valid in the direction from the base points to the turning point α. Remark also that U_0 is an exponentially decreasing solution with respect to h and that U_1 and U_2 are rightgoing and leftgoing waves respectively.

Now we set

$$U_0 = C_1 U_1 + C_2 U_2,$$

and we have

$$C_1 = \frac{[U_0, U_2]}{[U_1, U_2]}, \quad C_2 = \frac{[U_0, U_1]}{[U_2, U_1]}. \tag{14}$$

From the Wronskian formula (13), we get immediately

$$[U_1, U_2] = -\frac{2}{h} W^{+}_{\text{even}}(z_2; z_1, h), \quad [U_0, U_1] = \frac{2}{h} W^{+}_{\text{even}}(z_0; z_1, h). \tag{15}$$

For the calculation of $[U_2, U_0]$, we must be careful because of the cut. If we rewrite U_2 on the branch continued from x_0 to x_2 passing across the cut, we have

$$U_2 = -ie^{\pi i/4} w_+(x, h; \alpha, \hat{x}_2),$$

where $\hat{x}_2$ is the point x_2 on this new branch. Then writing $\hat{z}_2 = z(\hat{x}_2)$, we have

$$[U_2, U_0] = -\frac{2}{h} W^{+}_{\text{even}}(z_0; \hat{z}_2, h), \tag{16}$$

and we conclude that, using (14),

$$C_1 = -1 + O(h), \quad C_2 = 1 + O(h). \tag{17}$$

Similarly, we can treat the case where $Q(\beta) = 0$, $Q'(\beta) < 0$. We define three exact WKB solutions as above:

$$\begin{aligned} V_0 &= e^{-\pi i/4} w_+(x, h; \beta, y_0), \\ V_1 &= e^{+\pi i/4} w_-(x, h; \beta, y_1), \\ V_2 &= e^{-\pi i/4} w_+(x, h; \beta, y_2), \end{aligned}$$

and put

$$V_0 = D_1 V_1 + D_2 V_2.$$

Then we get as above

$$D_1 = 1 + O(h), \quad D_2 = 1 + O(h). \tag{18}$$

Notice that we could have written down much more precise results: Proposition 7 shows that we have a whole asymptotic expansion in powers of h for the above coefficients C_j or D_j in equations (17) and (18). In fact one can also prove *a priori* bounds on the coefficients of these expansions (they are classical analytic symbols), so that they can be summed to the lowest remainder (by the method of astronoms) (see [Ge-Gr]).

3 The Langer modification

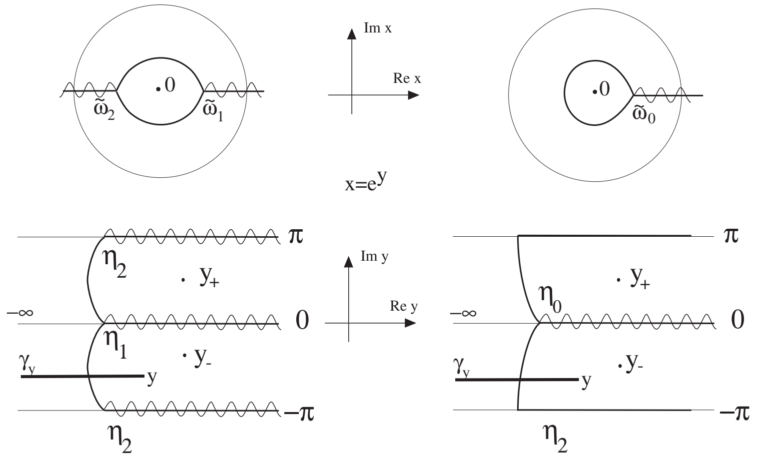
We want to study the behaviour of the solutions of equation (1) when both x and h go to 0. We recall that, compared with the case of the previous Section, the potential now depends on h and presents a double pole at the origin. As we said in Section 1, we first make the following change of variables:

$$\begin{cases} x = e^y, \\ x^{-1/2}u(x) = w(y), \end{cases} \tag{19}$$

and develop our exact WKB techniques for the new equation:

$$-h^2\frac{d^2w}{dy^2} + P(y,h)w = 0, \quad P(y,h) = e^{2y}V(e^y) + h^2(l+\frac{1}{2})^2. \tag{20}$$

In the strip $-\pi < \operatorname{Im} y \leq \pi$, this new equation presents in case (I) two turning points $\eta_{1,2}(h)$ which go away to $-\infty$ as $h \to 0$ since their real part is of order $\log h$. In case (II) there is one such turning point $\eta_0(h)$. Notice that they correspond now to zeros of the modified effective potential $\tilde{Q}$ under the map $x = e^y$.



I$_-$ ($q_{-1}=0$, $q_0<0$)

II$_-$ ($q_{-1}<0$)

Figure 3: Turning points and paths in the Langer plane.

We have drawn in Figure 3 the situation in the y-plane (called hereafter the Langer plane) in cases $(\mathrm{I})_-$ and $(\mathrm{II})_-$. For the sake of simplicity we will write the proofs below only in these cases, but the arguments run exactly in the same way in cases $(\mathrm{I})_+$ and $(\mathrm{II})_+$.

We want to construct exact WKB solutions in the Langer plane as in the previous section. It is important to notice that whereas the configuration of the Stokes lines to the left of the turning points is now quite simple (this is the main achievement of the Langer modification), this to the right of the turning points is really intricate. In particular it might be difficult to find a progressive path of infinite length as in [Ra], Section 3 (that is a path where $\mathrm{Re}\, z$ is strictly increasing, with a uniform positive lower bound on the rate of increase) in this region of the Langer plane.

In order to obtain the asymptotic behaviour of an exact WKB solution as $\mathrm{Re}\, y$ tends to $-\infty$ and h tends to 0, we take $y = -\infty$ as the base point for the symbol (which corresponds to x_1 in Section 2). As the base point for the phase, we choose the turning point $\eta(h)$ which by definition is $\eta_1(h)$ or $\eta_0(h)$ depending on the case $(\mathrm{I})_-$ or $(\mathrm{II})_-$, and we put

$$z(y,h) = \int_{\eta(h)}^{y} P(t,h)^{1/2} dt.$$

We place branch cuts as in Figure 3 and assume that $P(y,h)^{1/2}$ and $P(y,h)^{1/4}$ are positive for $y < \eta(h)$. Then $\mathrm{Re}\, z$ increases when $\mathrm{Re}\, y$ increases near $-\infty$ (see Figure 3). We shall show that the exact WKB solution

$$w^0(y,h) = e^{-\pi i/4} w_+(y,h;\eta(h),-\infty) \tag{21}$$

gives in the x-plane a solution which is of $O(x^{\ell+1})$ as x tends to the origin when $h > 0$ is fixed. We write this exact WKB solution (21) as (see (8) and (9))

$$w^0(y,h) = \frac{e^{-\pi i/4}}{P^{1/4}} e^{\int_\eta^y P^{1/2} dx/h} \{\sum_{n=0}^{\infty} (J \circ I_+)^n[1] - \sum_{n=0}^{\infty} I_+ \circ (J \circ I_+)^n[1]\}.$$

The essential step is to obtain suitable estimates for the operators $I_+[f]$ and $J[f]$:

$$\begin{aligned} I_+[f] &= \int_{\Gamma_z} e^{2(z_1 - z)/h} H(z_1,h) f(z_1,h) dz_1, \\ J[f] &= \int_{\Gamma_z} H(z_1,h) f(z_1,h) dz_1. \end{aligned} \tag{22}$$

The function $H(z,h)$ is defined by $H(z,h) = -P'_y(y,h)/(4P(y,h)^{3/2})$, and the integration path Γ_z in (22) is taken to be the image by $y \mapsto z(y,h)$ of $\gamma_y = \{y_1; -\infty < \mathrm{Re}\, y_1 < \mathrm{Re}\, y, \mathrm{Im}\, y_1 = \mathrm{Im}\, y\}$. We choose y with $0 < |\mathrm{Im}\, y| < \pi$ in case (I) and with $0 < |\mathrm{Im}\, y| < 2\pi$ in case (II) (see Figure 3), so that the path γ_y avoids the turning point(s) of P for all h's. In the Langer plane, we have

$$I_+[f] = -\frac{1}{4}\int_{\gamma_y} e^{-2\int_{y_1}^{y} P(y_2,h)^{1/2}dy_2/h} \frac{P'_y(y_1,h)}{P(y_1,h)} f\, dy_1,$$

$$J[f] = -\frac{1}{4}\int_{\gamma_y} \frac{P'_y(y_1,h)}{P(y_1,h)} f\, dy_1.$$

Notice here that $H(z_1,h)dz_1 = \{-P'_y(y_1,h)/4P(y_1,h)\}dy_1$ and that $-P'_y(y_1,h)/4P(y_1,h)$ is exponentially decreasing as $\mathrm{Re}\, y_1$ tends to $-\infty$ if $h > 0$. Hence the integrals in (22) are absolutely convergent when f is bounded for example.

We introduce new real variables r and θ by

$$r = \begin{cases} |e^y|/h, \\ |e^{y/2}|/h, \end{cases} \quad \theta = \begin{cases} \mathrm{Im}\, y & \text{in case (I)}, \\ \mathrm{Im}\, y/2 & \text{in case (II)}. \end{cases} \tag{23}$$

Since θ is constant on the integral contour, we can rewrite the integral operators I_+ and J in terms of r and h. Noticing that $dy_j = dr_j/r_j$ in case (I) (resp. $dy_j = 2dr_j/r_j$ in case (II)), we have

$$I_+[f](r,h) = \int_0^r e^{-\zeta(r,r_1,h)} K(r_1,h) f(r_1,h) dr_1, \tag{24}$$

$$J[f](r,h) = \int_0^r K(r_1,h) f(r_1,h) dr_1, \tag{25}$$

where

$$\zeta(r,r_1,h) = c_1 \int_{r_1}^{r} P^{1/2} \frac{dr_2}{r_2 h}, \quad K(r_1,h) = c_2 \frac{P'_y}{r_1 P}, \tag{26}$$

with $c_1 = 2$ (resp. 4) and $c_2 = -1/4$ (resp. $-1/2$). In terms of the variables (r,h), the functions P and P'_y are written as follows:

$$P(r_1,h) = h^2\{r_1^2 e^{2i\theta} V_0(hr_1e^{i\theta}) + (\ell+1/2)^2\}, \tag{27}$$

$$P'_y(r_1,h) = h^2 r_1^2 e^{2i\theta}\{2V_0(hr_1e^{i\theta}) + V_1(hr_1e^{i\theta})\}, \tag{28}$$

where

$$V_0(\xi) = \begin{cases} V(\xi), \\ \xi^2 V(\xi^2), \end{cases} \quad V_1(\xi) = \begin{cases} \xi V'_x(\xi) & \text{in case (I)}, \\ \xi^4 V'_x(\xi^2) & \text{in case (II)}. \end{cases}$$

Remark that

$$\lim_{\xi\to 0} V_0(\xi) = \begin{cases} q_0, \\ q_{-1}, \end{cases} \quad \lim_{\xi\to 0} V_1(\xi) = \begin{cases} 0 & \text{in case (I)}, \\ -q_{-1} & \text{in case (II)}. \end{cases}$$

We have the following lemmas:

Lemma 8 *Suppose that $\epsilon < |\theta| < \pi - \epsilon$ for a given positive ϵ. Then there exist positive δ and c such that for $e^{\mathrm{Re}\, y}$ $(= |x|) < \delta$, for any $y_1 \in \gamma_y$ and for any small h, we have in both cases*

$$Re\ P(r_1, h)^{1/2} \geq ch(1 + r_1).$$

Proof: Notice that the function $V_0(r_1, h)$ stays close to $q_0 < 0$ in case (I) and to $q_{-1} < 0$ in case (II) when $|x|$ is small. This means that there exists $\delta > 0$ such that if $|x| < \delta$, we have for all $h > 0$,

$$|\arg e^{2i\theta} V_0(r_1, h)| < \pi - \epsilon.$$

Since $(\ell + 1/2)^2$ is a positive constant, it is easy to see from (27) that $\mathrm{Re}\, P^{1/2}/h$ is bounded below by a positive constant.

Together with the fact that $\mathrm{Re}\, P^{1/2}/h$ behaves like $|\xi_1| = r_1$ as r_1 tends to $+\infty$, we get the Lemma. □

Lemma 9 *There exists a constant $C_1 > 0$ such that for any $y_1 \in \gamma_y$ and for any small h, we have in both cases,*

$$|P'_y(r_1, h)| \leq C_1 h^2 r_1^2.$$

Proof: From (28), we see that $|P'_y(r_1, h)|/h^2 r_1^2$ stays close to $2|q_0|$ in case (I) and to $|q_{-1}|$ and is bounded. □

Proposition 10 *Suppose that $\epsilon < |\theta| < \pi - \epsilon$ for a given positive ϵ. There exist positive constants δ, C and c such that if $e^{\mathrm{Re}\, y}$ $(= |x|) < \delta$, then in both cases $(I)_-$ and $(II)_-$ we have*

$$|(J \circ I_+)^n[1](r, h)| \leq \frac{C^{2n}}{2^n n!} (\frac{r}{1 + cr})^{4n}, \tag{29}$$

$$|I_+ \circ (J \circ I_+)^n[1](r, h)| \leq \frac{C^{2n+1}}{2^{n-1} n!} \frac{r^{4n+2}}{(1 + cr)^{4n+3}}. \tag{30}$$

Proof: We prove the estimate (29) by induction. It is obvious for $n = 0$, and we suppose it holds for n. For brevity we write $(J \circ I_+)^n[1] = p_n(y, h)$. It follows first from Lemma 8 and Lemma 9 (noticing also that $|P| \geq (\mathrm{Re}\, P^{1/2})^2$), that there exists $C > 0$ such that

$$|I_+[f]| \leq C e^{-cr} r^{-c} \int_0^r e^{cr_1} \frac{r_1^{c+1}}{(1 + r_1)^2} |f| dr_1,$$

and

$$|J[f]| \leq C \int_0^r \frac{r_1}{(1+r_1)^2}|f|dr_1,$$

where c is the same as in Lemma 8 and may be assumed to be smaller than 1. So we have

$$|I_+[p_n]| \leq \frac{C^{2n+1}}{2^n n!} e^{-cr} \int_0^r e^{cr_1} \frac{r_1^{4n+1}}{(1+cr_1)^{4n+2}} dr_1.$$

If we put $g(r) = e^{cr}\dfrac{r^{4n+2}}{(1+cr)^{4n+3}}$, we get

$$g'(r) = e^{cr}\frac{r^{4n+1}}{(1+cr)^{4n+2}}\frac{c^2r^2+4n+2}{(1+cr)^2},$$

so that

$$g'(r) \geq \frac{1}{2}e^{cr}\frac{r^{4n+1}}{(1+cr)^{4n+2}}$$

and

$$|I_+[p_n]| \leq \frac{C^{2n+1}}{2^{n-1}n!}\frac{r^{4n+2}}{(1+cr)^{4n+3}}. \tag{31}$$

Then we obtain

$$|J \circ I_+[p_n]| \leq \frac{C^{2n+2}}{2^{n-1}n!}\int_0^r \frac{r_1^{4n+3}}{(1+cr_1)^{4n+5}}dr_1 = \frac{C^{2n+2}}{2^{n+1}(n+1)!}(\frac{r}{1+cr})^{4(n+1)}.$$

and this completes the proof of (29). The estimate (30) follows immediately from (29) and (31). □

Theorem 1 follows easily from these estimates: we have by (29) and (30) that

$$(J \circ I_+)^n[1] = O(r^{4n}), \quad I_+ \circ (J \circ I_+)^n[1] = O(r^{4n+2}) \quad \text{as} \quad r \to 0. \tag{32}$$

Hence

$$\begin{aligned} x^{1/2}w^0(y,h) &= e^{-\pi i/4}e^{y/2}P^{-1/4}\exp(\textstyle\int^y P^{1/2}dt/h)(1+O(r^2)) \\ &= e^{-\pi i/4}\tilde{Q}^{-1/4}\exp(\textstyle\int^x \tilde{Q}^{1/2}dt/h)(1+O(r^2)), \end{aligned}$$

as r tends to 0 and in particular as x tends to 0 while $h > 0$ is fixed. Since $\tilde{Q} \sim h^2(\ell+1/2)^2/x^2$, the right hand side behaves like $x^{\ell+1}$. Therefore $x^{-1/2}w^0$ is proportional to u^0, and this gives Theorem 1.

Next we prove (4) of Theorem 2. We need two other exact WKB solutions: we choose two base points $y_\pm$ independent of h with $\theta = \theta_\pm = \pm\pi/2$ as in Figure 3. We set

$$\begin{aligned} w^+(y,h) &= e^{+\pi i/4} w_-(y,h;\eta(h),y_+),\\ w^-(y,h) &= e^{+\pi i/4} w_-(y,h;\eta(h),y_-). \end{aligned}$$

The point is that we know well the asymptotic form of these two exact WKB solutions on the real interval I. So it suffices to express w^0 in terms of w^+ and w^-, and Theorem 2 (4) follows from the following connection formula:

Proposition 11 *There exist two functions $A_+(h)$ and $A_-(h)$ and a positive number A satisfying*

$$A_+(h) = -A + o(1), \quad A_-(h) = A + o(1) \quad \textit{as} \quad h \to 0,$$

such that

$$w^0(y,h) = A_+(h) w^+(y,h) + A_-(h) w^-(y,h).$$

Proof: As in Section 2 (see (14) and (15)), we have

$$A_+(h) = -\frac{W^+_{\mathrm{even}}(z(y_-); z(-\infty), h)}{W^+_{\mathrm{even}}(z(y_-); z(\hat{y}_+), h)}, \quad A_-(h) = \frac{W^+_{\mathrm{even}}(z(y_+); z(-\infty), h)}{W^+_{\mathrm{even}}(z(y_-); z(\hat{y}_+), h)},$$

where $\hat{y}_+$ is, as in (16), the copy of the point y_+ on the other sheet of the Riemann surface. We have exactly as in Section 2 in spite of the dependence of P on h that

$$W^+_{\mathrm{even}}(z(y_-); z(\hat{y}_+), h) = 1 + O(h).$$

On the other hand, we need to study the behaviour as $h \to 0$ of $W^+_{\mathrm{even}}(z(y); z(-\infty), h)$ for fixed $y = y_\pm$. As above, we will consider this function of y and h as a function of r and h;

$$W^+_{\mathrm{even}}(z(y); z(-\infty), h) = \sum_{n=0}^{\infty} (J \circ I_+)^n [1](r,h). \tag{33}$$

We put for short $F(r,h) = \sum_{n=0}^{\infty} (J \circ I_+)^n [1](r,h)$. Applying the operator $J \circ I_+$ to both sides, we get

$$\begin{aligned} F(r,h) &= 1 + (J \circ I_+)[F](r,h)\\ &= 1 + \int \chi_{[0,r]}(r_1) K(r_1,h) I_+[F](r_1,h) dr_1 \end{aligned}$$

where $\chi_{[0,r]}$ is the characteristic function of the interval $[0, r]$, and K is the kernel defined in (26).

Now we show the existence of a limit for $F(r, h) = F(r(y, h), h)$ as h tends to 0. Recall that r is here a function of h defined by (23) with a fixed y.

First, it follows from the lemmas 8 and 9 that, for some positive constant M, $|K(r_1, h)| \leq Mr_1/(1 + r_1)^2$. We also have $|I_+[F](r_1, h)| \leq M'/(1 + cr_1)$ by (30), so that the function under the integral sign is dominated by an integrable function independent of h. Moreover for each fixed r_1, it is not difficult to see that $\chi_{[0,r_\pm]}(r_1)$, $K(r_1, h)$ and $I_+[F](r_1, h)$ have a limit as $h \to 0$, and the existence of a limit for $F(r, h)$ as h tends to 0 follows from Lebesgue's dominated convergence theorem. In particular if we take $y = y_\pm$, then we have

$$A_\pm = \lim_{h\to 0} F(r_\pm, h) = 1 + \int_0^\infty K_0(r_1) \sum_{n=0}^{\infty} I_+^0 \circ (J^0 \circ I_+^0)^n[1](r_1)dr_1, \quad (34)$$

where I_+^0 and J^0 are defined by (24) and (25) with

$$\zeta_0(r, r_1) = \zeta(r, r_1, 0) = \begin{cases} 2\int_{r_1}^{r} \{-q_0 r_2^2 + (\ell + 1/2)^2\}^{1/2} dr_2/r_2 \ (\mathrm{I})_-, \\ 4\int_{r_1}^{r} \{-q_{-1} r_2^2 + (\ell + 1/2)^2\}^{1/2} dr_2/r_2 \ (\mathrm{II})_-, \end{cases}$$

and

$$K_0(r_1) = K(r_1, 0) = \begin{cases} \dfrac{1}{2} \dfrac{q_0 r_1}{-q_0 r_1^2 + (\ell + 1/2)^2} & (\mathrm{I})_-, \\ \dfrac{1}{2} \dfrac{q_{-1} r_1}{-q_{-1} r_1^2 + (\ell + 1/2)^2} & (\mathrm{II})_-. \end{cases}$$

We then see that $A = A_+ = A_- > 1$. This completes the proof. □

4 Asymptotics of the actions

We prove now Corollary 4. We want to compute the Taylor expansion with respect to h of the h-dependent action integral in (4)

$$\Phi(h) = \int_{\tilde{\omega}}^{x_1} \sqrt{-\tilde{Q}} dt,$$

with $x_1 \in I$. As one would expect, the first term is easily seen to be the h-independent action integral $\int_0^{x_1} \sqrt{-V(x)}dx$. We need actually to compute also the second term since it gives the phase shift (see Corollary 4).

Recall that $\tilde{\omega}$ is one of $\tilde{\omega}_1$, $\tilde{\omega}_0$, which is the positive zero of $\tilde{Q}$ and that the integration path for $\Phi(h)$ lies on the positive real axis.

We work here under the assumption (A3), so that $\tilde{\omega}_2 = -\tilde{\omega}_1$. We are going to prove

Proposition 12 *For $x_1 \in I$, the function $\Phi(h)$ is holomorphic in a complex neighbourhood of $h = 0$ and*

$$\Phi(0) = \int_0^{x_0} \sqrt{-V(x)}dx, \quad \Phi'(0) = -\pi\lambda(\ell + 1/2),$$

where $\lambda = 1/2$ in case (I)$_-$ and $\lambda = 1$ in case (II)$_-$.

Proof: We take branch cuts for $\tilde{Q}^{1/2}$ and the integration paths as in Figure 4.

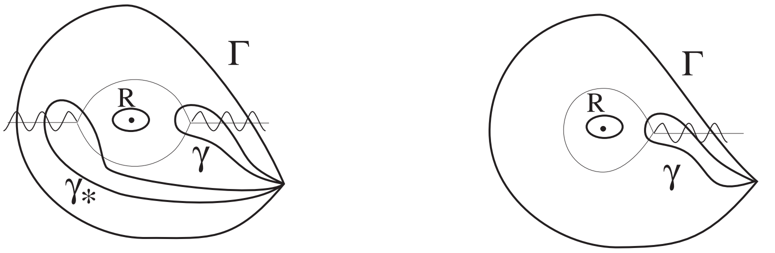


Figure 4: Integration paths.

The function $\tilde{Q}^{1/2}$ is assumed to be positive on the positive real axis near the origin. Then $2i\Phi(h) = \int_\gamma \tilde{Q}^{1/2}dx$ and

$$\int_\Gamma \tilde{Q}^{1/2}dx = \begin{cases} \int_\gamma \tilde{Q}^{1/2}dx + \int_{\gamma_*} \tilde{Q}^{1/2}dx + \int_R \tilde{Q}^{1/2}dx & \text{in case (I)}_-, \\ \int_\gamma \tilde{Q}^{1/2}dx + \int_R \tilde{Q}^{1/2}dx & \text{in case (II)}_-. \end{cases} \tag{35}$$

Let us write $L = \ell + 1/2$ for short. In both cases we have by the residue theorem

$$\int_R \tilde{Q}^{1/2}dx = 2\pi iLh.$$

We see also that $\int_\Gamma \tilde{Q}^{1/2}dx$ is holomorphic with respect to h^2 because Γ stays away from the zeros of $\tilde{Q}$ as h tends to 0. The proof in case (II)$_-$ is an immediate consequence of these facts.

In case (I)$_-$, moreover, we have $\int_\Gamma \tilde{Q}^{1/2}dx = 0$ thanks to the parity of V: indeed it reduces to -2-times the principal value of the integral of

$\sqrt{-x^2V(x)-L^2h^2}/x$ on the real interval $]-\tilde{\omega}_1, \tilde{\omega}_1[$, which is odd with respect to x. We also notice that

$$\Phi_*(e^{i\pi}h) = -\Phi(h),$$

where $2i\Phi_*(h) = \int_{\gamma_*} \tilde{Q}^{1/2}dx$. This can be checked by following the evolution of the integration path $\gamma_*(h)$ as h varies from h to $e^{i\pi}h$. Substituting $e^{i\pi}h$ in case $(\mathrm{I})_-$ of (35) we obtain

$$\Phi(e^{i\pi}h) - \Phi(h) - \pi Lh = 0, \tag{36}$$

and replacing h by $e^{i\pi}h$, we get also

$$\Phi(e^{2i\pi}h) - \Phi(e^{i\pi}h) + \pi Lh = 0.$$

Summing these two equalities, we see that the function $\Phi(h)$ is single-valued. Since it is bounded near the origin, $\Phi(h)$ is holomorphic there. Going back to (36), we obtain

$$\Phi(-h) - \Phi(h) - \pi Lh = 0,$$

which shows that the Taylor expansion of $\Phi(h)$ must be of the form

$$\Phi(h) = \Phi(0) - \frac{\pi}{2}Lh + O(h^2),$$

and this completes the proof. □

5 Application to barrier top resonances

We describe here briefly the results of [Fu-Ra 2] concerning barrier top resonances for the radial Schrödinger equation (1), which is the continuation of [Fu-Ra 1]. The complete proofs are to be found in [Fu-Ra 2]. We will suppose that V fulfills the following assumptions:

(H1) $V(x)$ is real on $\mathbb{R}_+$ and the function $x \mapsto xV(x)$ extends analytically to the domain

$$\mathcal{S} = \{x \in \mathbb{C}\backslash\{0\}; |\mathrm{arg}x| < \theta_0\} \cup \{x \in \mathbf{C}; |x| < R\}$$

for some $0 < \theta_0 < \pi/2$ and $R > 0$.

Notice that this assumption contains (A1). For the sake of simplicity we shall suppose that V is of short range, namely

(H2) There is an $\alpha > 0$ such that

$$V(x) = O(|x|^{-1-\alpha}) \quad \text{as} \quad |x| \to \infty \quad \text{in} \quad \mathcal{S}.$$

Concerning the shape of the physical potential, we will assume first that

(H3) V has a quadratic local maximum $V_m > 0$ on $]0, +\infty[$ at $x = m$. Moreover $V(x) < V_m$ for $x > m$.

and we will consider the following three different cases:

–**A.** There is an $\omega \in]0, m[$ such that $V(\omega) = V(m)$. In this case, we make the following further assumption:

(H4A) $V(x) > V(\omega)$ for $x \in [0, \omega[$, $V(x) < V(\omega)$ for $x \in]\omega, m[$ and $V'(\omega) < 0$.

–**B.** The function V has a global maximum at m, and is analytic in a vicinity of the origin.

–**C.** The function V has a global maximum at m and it has a coulomb-like singularity at the origin with negative residue.

Notice that in any case the effective potential $V(x) + h^2\ell(\ell+1)/x^2$ has the same shape for small positive h (see Figure 5).

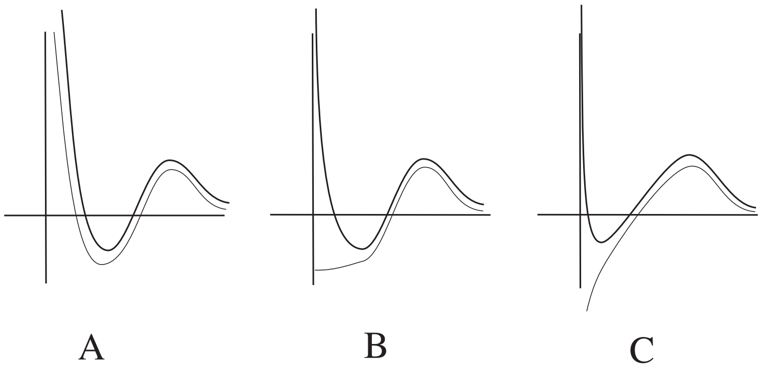


Figure 5: The effective and physical potentials.

Our aim is to calculate the scattering matrix near the critical energy level $E = V_m$ and to get quantization rules for the resonances close to V_m. Let us first recall what the scattering matrix and resonances for this operator are. Under our short-range assumption on V, the solutions of the radial Schrödinger equation behave as $x \to +\infty$ like

$$s_+(E,h)e^{i\sqrt{E}x/h} + s_-(E,h)e^{-i\sqrt{E}x/h}.$$

The scattering matrix is the ratio $\mathbf{S}_\ell(E,h) = -s_+(E,h)/s_-(E,h)$ corresponding to any non-trivial solution that goes to zero at the origin (see Section 1). This ratio is analytic with respect to E on the real axis and extends meromorphically in $\{E \in \mathbb{C}, -2\theta_0 < \arg(E - V_m) \leq 0\}$. The *resonances* are the poles of this meromorphic continuation.

Our method to compute the scattering matrix consists of constructing the WKB expansion of a solution which vanishes at the origin, so that we can compare it with the Jost solutions at infinity. Thus it is clear that the study of the preceeding sections should be our first step. The cases A, B and C correspond to the cases (I)$_\pm$ and (II)$_\pm$ as follows:

$$\begin{array}{l} A \leftrightarrow \text{case } (I)_+ \text{ and case } (II)_+ \\ B \leftrightarrow \text{case } (I)_-, \\ C \leftrightarrow \text{case } (II)_-. \end{array}$$

Let us first define h-independent action integrals associated with the physical potential $V(x)$. When $V_m - E$ is small and positive, there are in case (A) exactly three real zeros of $V(x) - E$: $0 < \omega(E) < \alpha(E) < \beta(E)$, and two zeros $0 < \alpha(E) < \beta(E)$ in cases (B) and (C). For such E's, we define

$$\begin{array}{l} \Sigma_1(E) = \int_{\alpha(E)}^{\beta(E)} \sqrt{V(x) - E}dx, \\ \Sigma_r(E) = \int_{\beta(E)}^{\infty} \{\sqrt{E} - \sqrt{E - V(x)}\}dx + \sqrt{E}\beta(E), \end{array}$$

and

$$\Sigma_{01}(E) = \begin{cases} \int_{\omega(E)}^{\alpha(E)} \sqrt{E - V(x)}dx & \text{in case (A)}, \\ \int_0^{\alpha(E)} \sqrt{E - V(x)}dx & \text{in cases (B) and (C)}, \end{cases}$$

where the square roots are assumed to be positive. Let us also define

$$\tilde{\Sigma}_{01}(E,h) = \Sigma_{01}(E) - \lambda(\ell + \frac{1}{2})\pi h.$$

where the number λ is defined by

$$\lambda = \begin{cases} 0 & \text{in case (A)}, \\ 1/2 & \text{in case (B)}, \\ 1 & \text{in case (C)}. \end{cases}$$

Denoting by $D(R)$ the complex disk of radius R with center at V_m and $\hat{D}(R)$ the universal covering of $D(R)\backslash\{V_m\}$, we can show as in [Fu-Ra 1] that the action integral Σ_1 extends analytically to $D(R)$ and Σ_{01} and Σ_r to $\hat{D}(R)$.

We obtain different expressions for the scattering matrix when E belongs to different domains in the (E,h)-complex space. In fact we use different techniques according to the distance between E and V_m. Moreover in the domain where $E - V_m$ is not of $O(h)$, the transition matrix at the barrier presents a Stokes phenomenon across the curve defined by $\mathrm{Re}\Sigma_1(E) = 0$ which is perpendicular to the real axis at V_0 (see [Fu-Ra 1]). Thus we will use the following notations:

$$\begin{aligned}
&D_1(R,r,h) = \hat{D}(R,]-\pi/2, \pi/2[)\backslash\hat{D}(rh),\\
&D_2(R,r,h) = \hat{D}(R,]-3\pi/2, -\pi/2[)\backslash\hat{D}(rh),\\
&D_3(r,h) = D(rh),
\end{aligned}$$

where we define for a real interval I,

$$\hat{D}(R,I) = \{E \in \hat{D}(R); \arg\Sigma_1(E) \in I\}.$$

Another function $N(z)$ plays an important role when the energy E is in the domain D_3. It is defined on the universal covering of $\mathrm{C}\backslash\{0\}$ by

$$N(z) = \frac{\sqrt{2\pi}}{\Gamma(1/2+z)} e^{z\log(z/e)}, \tag{37}$$

where $\log z$ is real when $\arg z = 0$. With these notations we have

Theorem 13 *Scattering matrix*
Let R be a sufficiently small positive number. Then there exist functions $\epsilon_j = \epsilon_j(E,h)$ $(1 \le j \le 12)$ analytic with respect to E with parameter h satisfying

$$\epsilon_j(E,h) = 1 + o(1) \quad (1 \le j \le 12)$$

such that the following formulas hold:

(i) There exists $r_0 > 0$ such that uniformly in any compact subset of $D_1(R, r_0, h)$ we have

$$\mathbf{S}_\ell(E,h) = ie^{-2i\Sigma_r/h}\frac{e^{2i\tilde{\Sigma}_{01}/h}\epsilon_1 + \epsilon_2}{e^{2i\tilde{\Sigma}_{01}/h}\epsilon_3 + \epsilon_4}, \tag{38}$$

and uniformly in any compact subset of $D_2(R, r_0, h)$ we have

$$\mathbf{S}_\ell(E,h) = ie^{-2i\Sigma_r/h}\frac{e^{-2\Sigma_1/h}e^{2i\tilde{\Sigma}_{01}/h}\epsilon_5 + \epsilon_6}{e^{2i\tilde{\Sigma}_{01}/h}\epsilon_7 + \epsilon_8}. \tag{39}$$

(ii) For any $r > 0$, we have uniformly in $D_3(r, h)$

$$\mathbf{S}_\ell(E, h) = ie^{-2i\Sigma_r/h} \frac{N(e^{-i\pi/2}\Sigma_1/\pi h)e^{2i\tilde{\Sigma}_{01}/h}\epsilon_9 + \epsilon_{10}}{e^{2i\tilde{\Sigma}_{01}/h}\epsilon_{11} + N(e^{i\pi/2}\Sigma_1/\pi h)\epsilon_{12}}. \qquad (40)$$

Recalling that resonances are the poles of the scattering matrix, we also get a quantization condition for the resonances in each domain of the energy plane:

Theorem 14 *Quantization conditions*
Suppose that E is a resonance in $D(R)$.

1. *If $E \in D_1(R, r_0, h) \cup D_2(R, r_0, h)$, then there is an $n \in \mathbb{N}$ such that*

$$\Sigma_{01}(E) = \{n + \frac{1}{2} + \lambda(\ell + \frac{1}{2})\}\pi h + o(h).$$

2. *If $E \in D_3(r, h)$, then there is an $n \in \mathbb{N}$ such that*

$$\Sigma_{01}(E) + i\frac{h}{2}\log N(i\frac{\Sigma_1(E)}{\pi h}) = \{n + \frac{1}{2} + \lambda(\ell + \frac{1}{2})\}\pi h + o(h).$$

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