Exponentially Accurate Semiclassical Tunneling Wave Functions in One Dimension

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Dedicated to the memory of our friend and colleague Pierre Duclos.

Abstract

We study the time behavior of wave functions involved in tunneling through a smooth potential barrier in one dimension in the semiclassical limit. We determine the leading order component of the wave function that tunnels. It is exponentially small in $1/\hbar$. For a wide variety of incoming wave packets, the leading order tunneling component is Gaussian for sufficiently small $\hbar$. We prove this for both the large time asymptotics and for moderately large values of the time variable.

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1 Introduction

The goal of this paper is to study the semiclassical limit of solutions to the one–dimensional time–dependent Schrödinger equation that involve tunneling through a simple potential barrier. Numerical simulations that illustrate our results are presented in [5]. A related wave packet "spawning" algorithm is also presented there.

Specifically, we consider solutions to

$$i\,\hbar\,\frac{\partial\Psi}{\partial t}\;=\;\left(-\,\frac{\hbar^2}{2}\,\frac{\partial^2}{\partial x^2}\;+\;V(x)\right)\Psi,\qquad\qquad \Psi(\cdot,\,t,\,\hbar)\in L^2(\mathbb{R}),\tag{1.1}$$

for small values of $\hbar$, where the potential V is an analytic function that represents a barrier. Our goal is to present formulas for the part of the wave function that has tunneled through the barrier.

1.1 A Qualitative Synopsis of our Results

Our results, stated in Theorems 2.4 and 2.5 and Corollary 2.6, are quite technical, so we begin with an informal, qualitative discussion of a special case.

Suppose $V(x)$ is a very simple, analytic bump function that tends sufficiently rapidly to zero as x tends to $+\infty$ and $-\infty$. For a wave coming in from the left, we choose generalized eigenfunctions that satisfy

$$\psi(k,\,x,\,\hbar)\quad\approx\quad\begin{cases} e^{ikx/\hbar}\;+\;R(k,\,\hbar)\;e^{-ikx/\hbar} & \text{as}\quad x\to-\infty\\ T(k,\,\hbar)\;e^{ikx/\hbar} & \text{as}\quad x\to+\infty,\end{cases}$$

with $k>0$.

We take superpositions of these, with energies below the top of the barrier V, to form wave packets and let them evolve. For a wide class of such superpositions, we have the following:

1. If the average momentum of the incoming wave packet is η, then the transition probability for tunneling is strictly greater than $|T(\eta,\,\hbar)|^2$.

2. The average momentum of the tunneling wave packet is strictly greater than η.

3. The leading term for the tunneling wave packet for small $\hbar$ is a complex Gaussian.

Our main results underpin the numerical spawning algorithm of [5] that describes semiclassical tunneling. The qualitative item 3 is crucial to the algorithm, whose quantitative information is determined numerically.

Intuitively, items 1, 2, and 3 are easy to understand. When $\hbar$ is small, the function $|T(k,\,\hbar)|$ increases extremely rapidly as k increases. For k near η, it typically grows like $C\ \exp(\alpha(k-\eta)/\hbar)$, with $\alpha>0$. Thus, higher momentum components of the wave packet are much more likely to tunnel than the average momentum components. Items 1 and 2 are consequences of this observation.

One can understand item 3 and learn more about item 2 by examining the transmitted wave packet in momentum space after tunneling has occurred. For example, if the incoming wave packet in momentum space is chosen to be asymptotic to one of the semiclassical wave packets ϕ_j of [6],

$$e^{-itk^2/(2\hbar)}\ 2^{-j/2}\ (j!)^{-1/2}\ \pi^{-1/4}\ \hbar^{-1/4}\ H_j((k-\eta)/\hbar^{1/2})\ \exp(-(k-\eta)^2/(2\,\hbar)),$$

then the transmitted wave packet behaves like

$$C\ \exp(\alpha(k-\eta)/\hbar)\, e^{-itk^2/(2\hbar)}\ 2^{-j/2}\ (j!)^{-1/2}\ \pi^{-1/4}\ \hbar^{-1/4}\ H_j((k-\eta)/\hbar^{1/2})\ \exp(-(k-\eta)^2/(2\,\hbar)).$$

This equals

$$e^{-itk^2/(2\hbar)}\ C\ e^{+\alpha^2/(2\hbar)}\ 2^{-j/2}\ (j!)^{-1/2}\ \pi^{-1/4}\ \hbar^{-1/4}\ H_j((k-\eta)/\hbar^{1/2})\ \exp(-(k-\eta-\alpha)^2/(2\,\hbar)),$$

The Gaussian factor is large only near $k=\eta+\alpha$, and near there, the Hermite polynomial behaves like its leading term, $2^j\ \alpha^j/\hbar^{j/2}$. This product is asymptotically another Gaussian with momentum near $\eta+\alpha$ for sufficiently small $\hbar$.

We note that the C in these expressions behaves like $e^{-K/\hbar}$, so none of this can be determined by a perturbation expansion in powers of $\hbar$.

To obtain quantitative results, we must insert energy cut offs and deal with many other technicalities, but the description above gives an intuitive summary of our results.

The precise statements of our results are presented in Section 2. Theorem 2.4 presents the very large time behavior of the tunneling wave function. Theorem 2.5 and Corollary 2.6 describe the behavior of the tunneling wave function for all times shortly after the tunneling has occurred.

2 A More Precise Description of the Problem

We consider wave packets that have their energy localized in an interval $\Delta = [E_1,\, E_2]$, and we assume the potential V satisfies the following hypotheses:

i) $x \mapsto V(x)$ is real analytic in the strip $S_\alpha = \{z : |\mathrm{Im}\, z| \le \alpha\}$, for some $\alpha > 0$.

ii) There exist $V(\pm\infty) \in (-\infty,\, E_1)$, $\nu > 1/2$, and $c < \infty$ such that

$$\limsup_{\mathrm{Re}\, z \to \pm\infty} \left(|\mathrm{Re}\, z|^{2+\nu} \sup_{|\mathrm{Im}\, z| \le \alpha} |V(z) - V(\pm\infty)| \right) \; < \; c. \tag{2.1}$$

iii) For any $E \in \Delta$, the function $V(x) - E$ has exactly two simple zeros, $x_0(E) < x_1(E)$ with $x_1(E) < 1$.

Under these hypotheses, we can decompose our solutions as superpositions of generalized eigenvectors of

$$H(\hbar) \;=\; -\,\frac{\hbar^2}{2}\,\frac{\partial^2}{\partial x^2} \;+\; V(x)$$

whose energy lies in Δ.

Since we are interested in the tunneling process, we assume that in the distant past, the wave packet was a scattering state, coming in from the left of the potential barrier. Our goal is to describe the leading order behavior of the wave packet on the right of the potential barrier for small $\hbar$ and sufficiently large positive times. This tunneling wave is well-known to have exponentially small norm in $1/\hbar$. We determine its leading order component and show that for a wide variety of incoming states, it is a Gaussian.

Analogous results for exponentially small reflected waves when the energy is strictly above a potential bump are presented in [2]. Similar results for non–adiabatic transitions in the Born–Oppenheimer approximation are presented in [8] and [11].

2.1 Generalized Eigenfunction Expansions

For any fixed energy $E < \max_{x \in \mathbb{R}} V(x)$, we let $\psi(x,\, E,\, \hbar)$ be the solution to the stationary Schrödinger equation

$$-\,\hbar^2\,\frac{\partial^2 \psi}{\partial x^2} \;=\; 2\,(E - V(x))\,\psi \;\equiv\; p^2(x,E)\,\psi, \tag{2.2}$$

that we construct below. Here,

$$p(x,\, E) \;=\; \sqrt{2\,(E - V(x))} \;>\; 0, \qquad \text{for} \qquad |x| \gg 1,$$

is the classical momentum at energy E. The turning points $x_0(E) < x_1(E)$, given by the two solutions of $p(x, E) = 0$ are branch points of $p(x, E)$, viewed as a multi-valued analytic function of x. We use the multivaluedness of this function in the analysis below.

We consider wave functions

$$\Psi(x, t, \hbar) \;=\; \int_\Delta Q(E, \hbar)\, e^{-itE/\hbar}\, \psi(x, E, \hbar)\, dE, \tag{2.3}$$

for some sufficiently regular energy density $Q(E, \hbar)$ defined on Δ. Such a function is a solution of (1.1) under the hypotheses we impose below on the energy density Q.

We shall derive a space–time description of the exponentially tunneling wave to leading order as $\hbar \to 0$ for large positive times, when this wave is far enough from the potential bump.

The energy densities $Q(E, \hbar)$ we choose are sharply peaked at a specific value $E_0 \in (E_1, E_2)$. Specifically, we consider

$$Q(E, \hbar) \;=\; e^{-G(E)/\hbar}\, e^{-iJ(E)/\hbar}\, P(E, \hbar), \tag{2.4}$$

where:

(C1) The real-valued function $G \geq 0$ is in $C^3(\Delta)$, is independent of $\hbar$, and has a unique non-degenerate minimum value of 0 at $E_0 \in (E_1, E_2)$. This implies that

$$G(E) \;=\; g\,(E - E_0)^2/2 \;+\; O\left((E - E_0)^3\right), \quad \text{where} \quad g > 0.$$

(C2) The real-valued function J is in $C^3(\Delta)$.

(C3) The complex-valued function $P(E, \hbar)$ is in $C^1(\Delta)$ and satisfies

$$\sup_{\substack{E \in \Delta \\ \varepsilon \geq 0}} \left| \frac{\partial^n}{\partial E^n} P(E, \hbar) \right| \;\leq\; C_n, \qquad \text{for} \qquad n = 0, 1.$$

2.2 The Specific Generalized Eigenfunction $\psi(x, E, \hbar)$

We first recast the eigenvalue problem for $H(\hbar)$ as a first order system of linear equations. We then use the analyticity of the potential and consider the extensions of these equations to the complex x-plane to perform our asymptotic analysis. The function $p(\cdot, E)$ has branch points at $x_0(E)$ and $x_1(E)$ which we have to select in a consistent way. Note the turning points $x_0(E) < x_1(E)$ are separated for all $E \in \Delta$.

We initially confine x to the real axis and define

$$p_R(x,\,E) \;=\; \sqrt{2\,|E - V(x)|} \;\geq\; 0. \tag{2.5}$$

We begin our analysis for $x > x_1(E)$, where $p_R(x,\,E)$ is the classical momentum.

Suppose ζ satisfies the ordinary differential equation (2.2). For $x > x_1(E)$, we define

$$\Phi(x) \;=\; \begin{pmatrix} \zeta(x) \\ i\,\hbar\,\zeta'(x) \end{pmatrix}, \tag{2.6}$$

where $'$ denotes the derivative with respect to x. We note that Φ satisfies

$$i\,\hbar\,\Phi'(x) \;=\; \begin{pmatrix} 0 & 1 \\ p^2(x,\,E) & 0 \end{pmatrix} \Phi(x) \;\equiv\; A(x,\,E)\;\Phi(x).$$

In order to apply the WKB method, we expand $\Phi(x)$ in terms of the instantaneous eigenvectors of the generator of $A(x,\,E)$. Specifically, we choose

$$\varphi_1(x) \;=\; \begin{pmatrix} \frac{1}{\sqrt{p_R(x,\,E)}} \\ \sqrt{p_R(x,\,E)} \end{pmatrix} \quad \text{and} \quad \varphi_2(x) \;=\; \begin{pmatrix} \frac{1}{\sqrt{p_R(x,\,E)}} \\ -\sqrt{p_R(x,\,E)} \end{pmatrix} \tag{2.7}$$

to be the eigenvectors associated with the eigenvalues $p_R(x,\,E)$ and $-p_R(x,\,E)$, respectively.

We decompose $\Phi(x)$ as

$$\Phi(x) \;=\; c_1(x)\; e^{-i\int_{x_1(E)}^{x} p_R(y,\,E)\,dy/\hbar}\;\varphi_1(x) \;+\; c_2(x)\; e^{i\int_{x_1(E)}^{x} p_R(y,\,E)\,dy/\hbar}\;\varphi_2(x), \tag{2.8}$$

where $c_1(x)$ and $c_2(x)$ are complex-valued coefficients that satisfy

$$\begin{pmatrix} c_1'(x) \\ c_2'(x) \end{pmatrix} \;=\; \frac{p_R'(x,\,E)}{2\,p_R(x,\,E)} \begin{pmatrix} 0 & e^{2i\int_{x_1(E)}^{x} p_R(y,\,E)\,dy/\hbar} \\ e^{-2i\int_{x_1(E)}^{x} p_R(y,\,E)\,dy/\hbar} & 0 \end{pmatrix} \begin{pmatrix} c_1(x) \\ c_2(x) \end{pmatrix} \tag{2.9}$$

These coefficients depend on E, and on sets where $p(x,\,E)$ is real-valued, they satisfy [12]

- $|c_1(x)|^2 - |c_2(x)|^2$ is independent of x, and
- $\begin{pmatrix} c_1(x) \\ c_2(x) \end{pmatrix}$ is a solution to (2.9) if and only if $\begin{pmatrix} \overline{c_1(x)} \\ \overline{c_2(x)} \end{pmatrix}$ is a solution to (2.9).

This decomposition allows us to write the solution to (2.2) for $x > x_1(E)$ as

$$\zeta(x,\,E,\,\hbar) \;=\; c_1(x,\,E,\,\hbar)\; e^{-i\int_{x_1(E)}^x p_R(y,\,E)\,dy/\hbar}\; \varphi_1^{(1)}(x,\,E,\,\hbar)$$

$$+\quad c_2(x,\,E,\,\hbar)\; e^{i\int_{x_1(E)}^x p_R(y,\,E)\,dy/\hbar}\; \varphi_2^{(1)}(x,\,E,\,\hbar), \tag{2.10}$$

where the E and $\hbar$ dependence is explicit, and $\varphi_j^{(1)}$ denotes the first component of φ_j.

When x is smaller than $x_0(E)$, so that the classical momentum again equals $p_R(x,E)$, a similar expansion is valid. However, we take a different phase convention when $x < x_0(E)$:

$$\zeta(x,\,E,\,\hbar) \;=\; d_1(x,\,E,\,\hbar)\; e^{-i\int_{x_0(E)}^x p_R(y,\,E)\,dy/\hbar}\; \varphi_1^{(1)}(x,\,E,\,\hbar)$$

$$+\quad d_2(x,\,E,\,\hbar)\; e^{i\int_{x_0(E)}^x p_R(y,\,E)\,dy/\hbar}\; \varphi_2^{(1)}(x,\,E,\,\hbar). \tag{2.11}$$

where the coefficients d_1 and d_2 satisfy a differential equation similar to (2.9).

We need to connect the coefficients c_1 and c_2 to the coefficients d_1 and d_2. One commonly used technique consists of solving a similar equation for $x_0(E) < x < x_1(E)$ and matching the solutions to those we just described. Instead we use the complex WKB method which allows us to work with just one equation, but requires an analytic framework. See [1] for various possible approaches.

We only want to have an outgoing wave on the right and are not currently worrying about normalization, so we consider the asymptotic conditions

$$c_1(+\infty,\,E,\,\hbar) \;=\; 0, \qquad \text{and} \qquad c_2(+\infty,\,E,\,\hbar) \;=\; 1. \tag{2.12}$$

Then as in [8] and [11], we have

$$p_R(\pm\infty,\,E) \;>\; 0,$$

$$\varphi_j(\pm\infty,\,E) \;=\; \begin{pmatrix} \frac{1}{\sqrt{p_R(\pm\infty,\,E)}} \\ (-1)^{j+1}\,\sqrt{p_R(\pm\infty,\,E)} \end{pmatrix},$$

$$\int_{x_1(E)}^x p_R(y,\,E)\,dy \;=\; (x-x_1(E))\;p_R(\infty,\,E) \;+\; \int_{x_1(E)}^{\infty} (p_R(y,\,E)-p_R(\infty,\,E))\,dy$$

$$+\quad O\left(|x|^{-1-\nu}\right), \qquad \text{as} \quad x\to\infty, \qquad\qquad \text{and}$$

$$\int_{x_0(E)}^x p_R(y,\,E)\,dy \;=\; (x-x_0(E))\;p_R(-\infty,\,E) \;+\; \int_{x_0(E)}^{-\infty} (p_R(y,\,E)-p_R(-\infty,\,E))\,dy$$

$$+ \quad O\left(|x|^{-1-\nu}\right) \qquad \text{as} \quad x \to -\infty.$$

The error estimates here are uniform for $E \in \Delta$.

We thus have an incoming wave asymptotically described for large negative x by

$$d_2(-\infty,\, E,\, \hbar)\ \frac{e^{i\int_{x_0(E)}^{-\infty}(p_R(y,E)-p_R(-\infty,E))\,dy/\hbar}}{\sqrt{p_R(-\infty,\, E)}}\ e^{-ip_R(-\infty,E)x_0(E)/\hbar}\ e^{i\,p_R(-\infty,E)\,x/\hbar}.$$

The reflected wave is asymptotically described for large negative x by

$$d_1(-\infty,\, E,\, \hbar)\ \frac{e^{-i\int_{x_0(E)}^{-\infty}(p_R(y,E)-p_R(-\infty,E))\,dy/\hbar}}{\sqrt{p_R(-\infty,\, E)}}\ e^{+ip_R(-\infty,E)x_0(E)/\hbar}\ e^{-\,i\,p_R(-\infty,E)\,x/\hbar}.$$

The transmitted wave is asymptotically described for large positive x by

$$\frac{e^{i\int_{x_1(E)}^{+\infty}(p_R(y,E)-p_R(+\infty,E))\,dy/\hbar}}{\sqrt{p_R(\infty,\, E)}}\ e^{-ip_R(-\infty,E)x_1(E)/\hbar}\ e^{i\,p_R(+\infty,E)\,x/\hbar}. \tag{2.13}$$

We obtain the solution $\psi(x,\, E,\, \hbar)$ that we use in (2.3) by normalizing the incoming flux. To do so, we simply divide the whole solution $\zeta(x,\, E,\, \hbar)$ by the constant

$$d_2(-\infty,\, E,\, \hbar)\ \frac{e^{i\int_{x_0(E)}^{-\infty}(p_R(y,E)-p_R(-\infty,E))\,dy/\hbar}}{\sqrt{p_R(-\infty,\, E)}}\ e^{-ip_R(-\infty,E)x_0(E)/\hbar}.$$

We obtain our main results by analyzing the tunneling wave by studying the large x and t asymptotics of (2.3) with this $\psi(x,\, E,\, \hbar)$ and an any appropriate choice of $Q(E,\, \hbar)$.

2.3 Complex WKB analysis

We need to compute the asymptotic behavior, as $x \to -\infty$, of the solution to (2.9) that satisfies (2.12). We do this by applying the complex WKB method in order to avoid matching of the solutions at the real turning points $x_0(E)$ and $x_1(E)$, where the equation is ill-defined. So, we consider (2.2) and (2.9) in the strip S_α in the complex plane containing the real axis, with possible branch cuts at $x_0(E)$ and $x_1(E)$. We now replace the variable x by z, to emphasize that the variable is no longer restricted to the real line. The solution to (2.2) is analytic for $z \in S_\alpha$, but the solution to (2.9) has singularities at the turning points. As $\mathrm{Re}\, z$ tends to $+\infty$ in S_α, our assumptions on the behavior of the potential ensure that the asymptotic values of the coefficients $c_j(z)$ are independent of $\mathrm{Im}\, z$. We can thus start the integration of (2.9) above the real axis at the extreme right of the strip, with asymptotic boundary data (2.12). Also, our assumptions imply the existence of two C^1 paths from the right end of the strip S_α to its left end, with one of them, γ_a, passing above the two turning points, and the other, γ_b, passing between them. We parameterize these with $t \in \mathbb{R}$ and assume they satisfy

$$\gamma_\#(t) \in S_\alpha, \qquad \text{with} \qquad \lim_{t \to \pm\infty} \operatorname{Re} \gamma_\#(t) \ = \ \mp\infty, \qquad \text{and} \qquad \sup_{t \to \pm\infty} |\dot{\gamma}_\#(t)| \ < \ \infty,$$

where $\#$ stands for a or b. See Figures 1, 2, and 3 for descriptions of the relevant Stokes Lines, Anti–Stokes Lines, and the specific paths that we choose. Note that $\operatorname{Im} \gamma_a(t) > 0$ for all t, whereas $\operatorname{Im} \gamma_b$ changes sign exactly once and is positive for t large and negative. Finally, and this is the main property of these paths, the imaginary part of $\int_{x_1(E)}^z p(z',\, E)\, dz'$ along $\gamma_\#$ is decreasing. Such paths are called dissipative.

The existence of these dissipative paths is proved as in [10] and [9]. Close enough to the real axis, there exist level lines of the function $\operatorname{Im} \int_{x_1(E)}^z p(z',\, E)\, dz'$ which are essentially parallel to the real axis for $\operatorname{Re} z \geq x_1(E)$ and $\operatorname{Re} z \leq x_0(E)$. For $x_0(E) \leq \operatorname{Re} z \leq x_1(E)$, these lines can be connected by means of level lines of $\operatorname{Re} \int_{x_1(E)}^z p(z',\, E)\, dz'$, along which $\operatorname{Im} \int_{x_1(E)}^z p(z',\, E)\, dz'$ is strictly decreasing. As a local analysis reveals, the connections can be made in a C^1 fashion without losing the dissipativity property. It is readily seen by inspection, that γ_a can be constructed this way. For γ_b, one starts as for γ_a, and between $x_0(E)$ and $x_1(E)$, one uses a level line of $\operatorname{Im} \int_{x_1(E)}^z p(z',\, E)\, dz'$ to cross the real axis. Then one connects to a level line of $\operatorname{Re} \int_{x_1(E)}^z p(z',\, E)\, dz'$ and proceeds as described above to connect to $-\infty$ below the real axis.

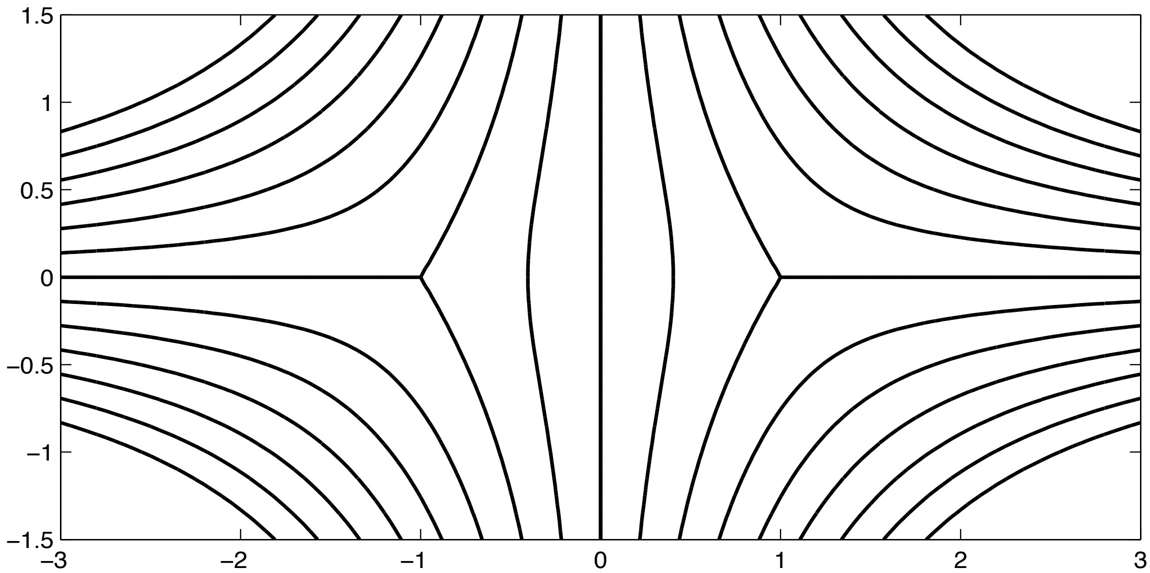

Figure 1. Stokes Lines, along which $\operatorname{Im} \int_{x_1(E)}^z p(z',\, E)\, dz'$ is constant

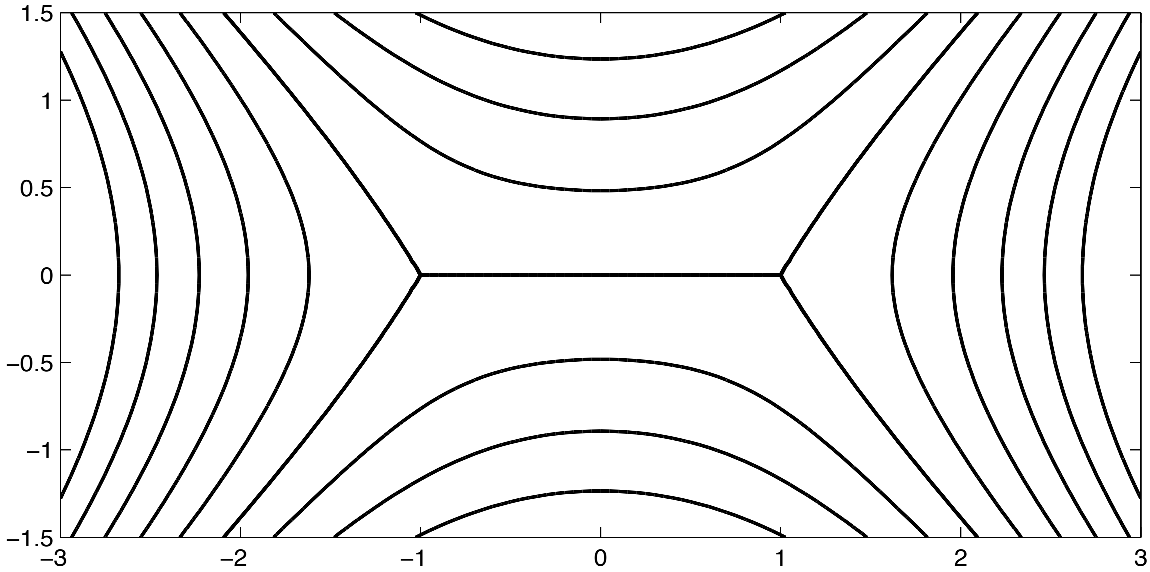

Figure 2. Anti–Stokes Lines, along which $\text{Re} \int_{x_1(E)}^{z} p(z',\, E)\, dz'$ is constant

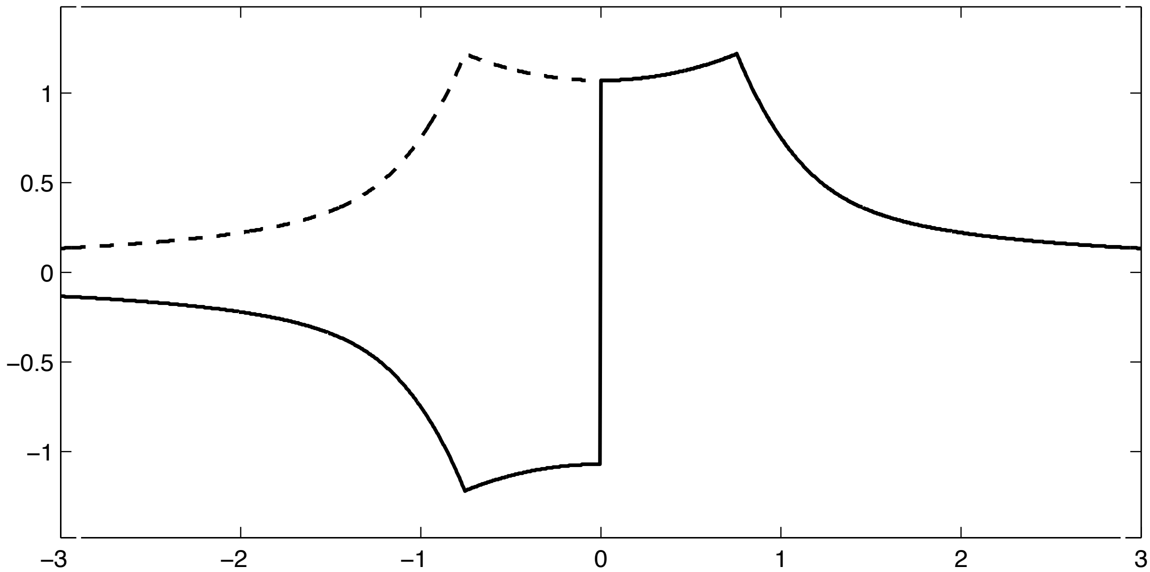

Figure 3. The Paths γ_a (dashed line) and γ_b, (solid line).

We can integrate (2.9) along these two different paths and compare the solutions for large negative $\text{Re}\, z$ with $z \in S_\alpha$. These two integrations describe the same solution to (2.2) since it is analytic. Moreover, the asymptotic values of the coefficients as $\hbar \to 0$ can be controlled, because both these paths are dissipative.

We choose two specific branches, $p^a(z,\, E)$ and $p^b(z,\, E)$, of the multivalued function $p(z,\, E)$. For $p^a(z,\, E)$ we place vertical branch cuts below the real axis, extending down from $x_0(E)$ and $x_1(E)$. For $p^b(z,\,E)$ we place a vertical branch cut below the real axis extending down from $x_1(E)$, and a vertical branch cut above the real axis extending up from $x_0(E)$. These two functions are then uniquely determined in their respective regions S^a_α and S^b_α by the requirement that they both equal $p_R(z,\,E)$ when z is real and greater than $x_1(E)$.

The following are satisfied when z is on the real axis:

$$p^a(x,\,E) \quad = \quad \begin{cases} p_R(x,\,E) \ > \ 0, & \text{if} \quad x > x_1(E) \\ e^{i\pi/2}\,p_R(x,\,E), & \text{if} \quad x_0(E) < x < x_1(E) \\ -\,p_R(x,\,E) \ < \ 0, & \text{if} \quad x < x_0(E). \end{cases}$$

and

$$p^b(x,\,E) \quad = \quad \begin{cases} p_R(x,\,E) \ > \ 0, & \text{if} \quad x > x_1(E) \\ e^{i\pi/2}\,p_R(x,\,E), & \text{if} \quad x_0(E) < x < x_1(E) \\ p_R(x,\,E) \ > \ 0, & \text{if} \quad x < x_0(E). \end{cases}$$

For $\#=a,\,b,$ the function $p^{\#}(z,\,E)$ is analytic in a neighborhood of the path $\gamma_{\#}$.

We define $\varphi^{\#}_j(z,\,E),$ to be the analytic continuation in $S^{\#}_\alpha$ of the vector $\varphi_j(z,\,E)$ defined in (2.7). We also define $\displaystyle\int_{x_1(E)}^{z} p^{\#}(y,\,E)\,dy$ to be the analytic continuation in $S^{\#}_\alpha$ of $\displaystyle\int_{x_1(E)}^{z} p(y,\,E)\,dy,$ which is already specified for $x > x_1(E)$.

Lemma 2.1 *For any real* $z < x_0(E),$ *the following are satisfied:*

$$i\,\varphi^a_1(z) \ = \ \varphi^b_2(z) \ = \ \begin{pmatrix} \frac{1}{\sqrt{p_R(z,\,E)}} \\ -\,\sqrt{p_R(z,\,E)} \end{pmatrix},$$

$$i\,\varphi^a_2(z) \ = \ \varphi^b_1(z) \ = \ \begin{pmatrix} \frac{1}{\sqrt{p_R(z,E)}} \\ \sqrt{p_R(z,\,E)} \end{pmatrix},$$

$$\int_{x_1(E)}^{z} p^b(y,\,E)\,dy \ = \ i\int_{x_1(E)}^{x_0(E)} p_R(y,\,E)\,dy \ + \ \int_{x_0(E)}^{z} p_R(y,\,E)\,dy \tag{2.14}$$

$$\int_{x_1(E)}^{z} p^a(y,\,E)\,dy \ + \ \int_{x_1(E)}^{z} p^b(y,\,E)\,dy \ = \ -\,2\,i\int_{x_0(E)}^{x_1(E)} p_R(y,\,E)\,dy.$$

Proof We simply follow the analytic continuations of p in the respective domains. ■

Remarks

i) The quantity $2\int_{x_0(E)}^{x_1(E)} p_R(y,\, E)\, dy$ can be expressed as a contour integral

$$K(E) \;=\; 2\int_{x_0(E)}^{x_1(E)} p_R(y,\, E)\, dy \;=\; \int_\gamma p(z,\, E)\, dz \;>\; 0,$$

where γ is a simple negatively oriented loop around the two turning points, and $p(z,\, E)$ is the analytic continuation of $p_R(x,\, E)$ for $x > x_0(E)$. This shows that $K(E)$ is analytic for E in a complex neighbourhood of the energy window Δ.

ii) Equation (2.14) shows that the analytic continuations $(c_1^b(z),\, c_2^b(z))$ of the coefficients coincide with $(d_1(z),\, d_2(z))$ in (2.11) for $z < x_0(E)$, up to multiplicative constants.

Coming back to the differential equation (2.9), we denote the analytic continuations of its solutions in $S_\alpha^\#$ as $(c_1^\#, c_2^\#)$. We consider the analytic function Φ for $z < x_0(E)$ and the two different analytic continuations of its decomposition (2.8) at z. These two representations must agree. This and Lemma 2.1 imply the following:

Lemma 2.2 *For any $z < x_0(E)$, we have*

$$i\, c_2^b(z,\, E,\, \hbar)\, e^{K(E)/\hbar} \;=\; c_1^a(z,\, E,\, \hbar)$$

$$i\, c_1^b(z,\, E,\, \hbar)\, e^{-K(E)/\hbar} \;=\; c_2^a(z,\, E,\, \hbar).$$

Remark The identities in the two previous lemmas are actually true for any z with $\mathrm{Re}\, z < x_0(E)$.

The WKB analysis of (2.9) along the dissipative paths $\gamma^\#$ and assumption (2.1) now yield the following lemma, as shown in [10], [9], [8], [11].

Lemma 2.3 *We have*

$$c_2^a(-\infty,\, E,\, \hbar) \;=\; 1 \;+\; O_E(\hbar), \qquad \text{as} \quad \hbar \to 0,$$

$$c_2^b(-\infty,\, E,\, \hbar) \;=\; 1 \;+\; O_E(\hbar), \qquad \text{as} \quad \hbar \to 0, \qquad \text{and}$$

$$c_j^\#(x,\, E,\, \hbar) \;=\; c_j^\#(\pm\infty,\, E,\, \hbar) \;+\; O_E(1/|x|^{1+\nu}) \qquad \text{as} \quad x \to \pm\infty,$$

where the remainder terms are analytic in E, *for* E *in a complex neighborhood of the real set* Δ. *Moreover,* $\frac{d}{dE}\, c_2^b(-\infty,\, E,\, \hbar)$ *and the* $O_E(1/|x|^\nu)$ *are uniformly bounded as* $\hbar \to 0$.

As a consequence of this lemma, for $x \gg 1$, we have

$$\zeta(x,\, E,\, \hbar) \;=\; \frac{e^{i(\int_{x_1(E)}^{\infty} (p_R(y,\,E)-p_R(\infty,\,E)\,dy)/\hbar}\; e^{-ix_1(E)p_R(\infty,\,E)/\hbar}}{\sqrt{p_R(\infty,\, E)}}\quad e^{i\,p_R(+\infty,\,E)\,x/\hbar}$$
$$\times\quad \left(1 + O_E(\hbar) \;+\; O_E(1/(\hbar\,|x|^{1+\nu})\right)$$

and, for $x \ll -1$, we have

$$\begin{aligned}\zeta(x,\, E,\, \hbar) \;&=\; -\,i\; e^{K(E)/(2\hbar)}\; \frac{e^{i(\int_{-\infty}^{x_0(E)}(p_R(s,E)-p_R(-\infty,E)ds)/\hbar}\; e^{ix_0(E)p_R(-\infty,E)/\hbar}}{\sqrt{p_R(-\infty,\, E)}}\; e^{-\,i\,p_R(-\infty,\,E)\,x/\hbar}\\ &\quad+\; e^{K(E)/(2\hbar)}\; \frac{e^{-i(\int_{-\infty}^{x_0(E)}(p_R(s,E)-p_R(-\infty,E)ds)/\hbar}\; e^{-ix_0(E)p_R(-\infty,E)/\hbar}}{\sqrt{p_R(-\infty,\, E)}}\; e^{i\,p_R(-\infty,\,E)\,x/\hbar}\\ &\quad+\; e^{K(E)/(2\hbar)}\; \left(\, e^{i\,p_R(-\infty,\,E)\,x/\hbar} \;+\; e^{-\,i\,p_R(-\infty,E)\,x/\hbar}\,\right)\\ &\qquad\times\; \left(O_E(\hbar) \;+\; O_E(1/(\hbar\,|x|^{1+\nu})\right). \end{aligned} \tag{2.15}$$

2.4 Large Time Asymptotics of the Tunneling Wave Function

We now consider the large time behavior of the transmitted wave packet. We denote this wave packet by $\chi(x,\, t,\, \hbar)$. We construct it as a time-dependent superposition of the normalized generalized wave functions $\psi(x,\, E,\, \hbar)$, where $x > 1 > \max\limits_{E\in\Delta}\, x_1(E)$.
The specific superposition we use is

$$\chi(x,\, t,\, \hbar) \;=\; \int_\Delta\, Q(E,\, \hbar)\; e^{-\,i\,t\,E/\hbar}\; \psi(x,\, E,\, \hbar)\; dE, \tag{2.16}$$

where for $x > \max\limits_{E\in\Delta}\, x_1(E)$,

$$\begin{aligned}&\psi(x,\, E,\, \hbar) \\ &=\; \frac{e^{-K(E)/(2\hbar)}\;\; \sqrt{p(-\infty,\, E)}\;\; c_2^a(x,\, E,\, \hbar)\;\; e^{i\int_{x_1(E)}^{x}\, p_R(y,\,E)\,dy/\hbar}}{\sqrt{p(x,\, E)}\;\; c_2^b(-\infty,\, E,\, \hbar)\;\; e^{-i\int_{-\infty}^{x_0(E)}(p_R(y,E)-p_R(-\infty,E))/\hbar}\;\; e^{-\,i\,p_R(-\infty,\,E)\,x_0(E)}}\,. \end{aligned} \tag{2.17}$$

See Remark ii) after Lemma 2.1. The asymptotics we have established show that for large positive x,

$$\chi(x,\,t,\,\hbar)\;=\;\int_\Delta\,Q(E,\,\hbar)\,\sqrt{\frac{p(-\infty,\,E)}{p(+\infty,\,E)}}\;e^{-K(E)/(2\hbar)}\;e^{i\,(p_R(\infty,\,E)\,x\,-\,E\,t)/\hbar}$$

$$\times\quad e^{-\,i\,\omega(E)/\hbar}\quad(\,1\,+\,r(x,\,E,\,\hbar)\,)\;\;dE,$$

where

$$\omega(E)\;=\;-\,\int_{x_1(E)}^{\infty}(p_R(y,\,E)-p_R(\infty,\,E))\,dy\;-\;\int_{-\infty}^{x_0(E)}(p_R(y,\,E)-p_R(-\infty,\,E))\,dy$$

$$+\;\;p_R(-\infty,\,E)\,(x_1(E)-x_0(E)).$$

The error term $r(x,\,E,\,\hbar)$ in this expression satisfies

$$r(x,\,E,\,\hbar)\;=\;O\left(\hbar\,+\,\frac{1}{\hbar\,|x|^{1+\nu}}\,+\,\frac{1}{|x|^{2+\nu}}\right)\;=\;O\left(\hbar\,+\,\frac{1}{\hbar\,|x|^{1+\nu}}\right),$$

uniformly for $E\in\Delta$, $x>1$ and $\hbar$ small enough.

We prove below that $\chi(x,\,t,\,\hbar)$ asymptotically propagates freely to the right for large positive t.

For $E\in\Delta$, we define

$$\alpha(E)\;=\;G(E)\;+\;K(E)/2\qquad\text{and}\qquad\kappa(E)\;=\;J(E)\;+\;\omega(E),\tag{2.18}$$

where G and J are the functions in (2.4). We then have

$$\chi(x,\,t,\,\hbar)\tag{2.19}$$

$$=\;\int_\Delta\,P(E,\hbar)\,\sqrt{\frac{p(-\infty,\,E)}{p(+\infty,\,E)}}\;e^{-\alpha(E)/\hbar}\;e^{-\,i\,\kappa(E)/\hbar}\;e^{i\,(p_R(\infty,\,E)\,x\,-\,E\,t)/\hbar}\,(1\,+\,r(x,\,E,\,\hbar))\;dE.$$

We obtain the small $\hbar$ asymptotics of this integral by Laplace's method. We first state a result concerning the large x and large t behavior of $\chi(x,\,t,\,\hbar)$, whose proof follows from the methods of [8] and [11], but is easier. The detailed analysis of the x and t dependence yields the following result. See [8] and [11] for details.

Theorem 2.4 *Assume the function $\alpha(E)$ has a unique non-degenerate minimum at $E=E^*$ in Δ. Define $k(E)=p_R(\infty,\,E)$ and $k^*=k(E^*)$.*

There exist $\delta > 0$ *and* $T_\hbar > 0$, *such that for* $t > T_\hbar$ *and all* $x > 1$, *the transmitted wave satisfies*

$$\chi(x,\,t,\,\hbar) \quad = \quad \chi^{\infty}_{Gauss}(x,\,t,\,\hbar) \;+\; O\left(e^{-\,\alpha(E^*)/\hbar}\,\hbar^{3/4+\delta}\right),$$

where the error term is measured in the L^2 *norm, uniformly for* $t > T_\hbar$, *and*

$$\begin{aligned}\chi^{\infty}_{Gauss}(x,t,\hbar) \quad &= \quad \sqrt{2\,\pi\,\hbar\,k^*}\;\; P(E^*,\,\hbar)\;\sqrt{\frac{p(-\infty,\,E^*)}{p(+\infty,\,E^*)}}\;\; e^{-\,\alpha(E^*)/\hbar} \\ &\times \quad \frac{\exp\{\,-\,i\,(t\,E^*\,+\,\kappa(E^*)\,-\,k^*\,x)/\hbar\,\}}{\left(\,\frac{d^2}{dk^2}\,\alpha(E(k))|_{k^*}\,+\,i\,(\,t\,+\,\frac{d^2}{dk^2}\,\kappa(E(k))|_{k^*}\,)\,\right)^{1/2}} \\ &\times \quad \exp\left\{-\,\frac{(x\,-\,k^*(t+\kappa'(E^*)))^2}{2\,\hbar\,\left(\,\frac{d^2}{dk^2}\,\alpha(E(k))|_{k^*}\,+\,i\,(\,t\,+\,\frac{d^2}{dk^2}\,\kappa(E(k))|_{k^*}\,)\,\right)}\right\}.\end{aligned}$$

Proof Outline The proof of this theorem is very technical, but is very similar to ones presented for Theorem 5.1 of [8] and Theorem 6 of [11]. One computes the leading term $\chi^{\infty}_{Gauss}(x,\,t,\,\hbar)$ by a rigorous version of Laplace's method, paying attention to the dependence of the remainder terms on the parameters x and t. The L^2 norm of this leading term is

$$\hbar^{3/4}\;\pi^{3/4}\;\sqrt{2\,k^*}\;\; e^{-\,\alpha(E^*)/\hbar}\;\; P(E^*,\hbar)\;\sqrt{\frac{p(-\infty,\,E^*)}{p(+\infty,\,E^*)}}\;\;\left(\left.\frac{d^2}{dk^2}\right|_{k=k^*}\alpha(E(k))\right)^{-1/4}, \qquad (2.20)$$

which is $O\left(\hbar^{3/4}\,e^{-\,\alpha(E^*)/\hbar}\right)$. By the methods of used in [8] and [11], the L^2 norm of the error term induced by $r(x,\,E,\,\hbar)$ under the integral sign in (2.19) is of order $\hbar^{3/4+\delta}\,e^{-\alpha(E^*)}$, for some $\delta > 0$, provided t is large enough. Note that Lemma 1 and Proposition 5 of [2] allow us to get better control of $T_\hbar$. (See below.) ■

2.5 The Transmitted Wave Function Shortly After Tunneling

Mimicking [2], we shall now address the behavior of the transmitted wave for finite values of x and t, shortly after the transmitted wave has left the region where it emerges from the potential barrier. Because the exponential decay of transmitted wave computed from the behavior of $p(z,E)$ on the real axis appears as a factor, see (2.17), the analysis of the semicassical behavior of the coefficient $c^a(x,\,E,\,\hbar)$ for finite values of $x > x_1(E)$ is simpler than in [2]. By contrast, the appearance for finite x's of the corresponding exponentially small factor for the above barrier reflection required to pass to the superadiabatic representation in [2]. This is not necessary here so that we can stick to the adiabatic basis (2.10). We shall not, however, examine the more delicate details of how the transmitted wave actually emerges from the barrier. One should be able to address this much more technical topic by adapting the results of [2].

Let

$$\rho(E) \;=\; -\int_{-\infty}^{x_0(E)} (p_R(y,\,E)\;-\;p_R(-\infty,\,E))\,dy \quad - \quad p_R(-\infty,\,E)\;x_0(E),$$

$$S(x,\,t,\,E) \;=\; -\int_{x_1(E)}^{x} p_R(y,E)\,dy \;+\; \rho(E) \;+\; J(E) \;+\; E\,t,$$

and

$$P_0(x,\,E) \;=\; \frac{P(E,\,\hbar)\,\sqrt{p_R(-\infty,\,E)}}{\sqrt{p_R(x,\,E)}}.$$

In the region of moderately large positive x, but far from the potential barrier, the transmitted wave is described by the following theorem, which requires faster decay of the potential to its asymptotic value.

Theorem 2.5 *Let $\nu > 21/2$. There exist $\delta > 0$, $\tau > 0$, $C > 0$, and $\beta > 0$, such that for all $t > \tau$ and sufficiently small $\hbar$,*

$$\chi(x,\,t,\,\hbar) \;=\; \left\{ \begin{array}{ll} \chi_{mod}(x,\,t,\,\hbar) & \text{if} \;\; 1 < x < C\hbar^{-\beta} \\ \chi^{\infty}_{Gauss}(x,t,\hbar) & \text{if} \;\; C\hbar^{-\beta} \le x \\ 0 & \text{otherwise} \end{array} \right\} \;+\; O\left(\hbar^{3/4+\delta}\,e^{-\alpha(E^*)/\hbar}\right),$$

where the error term is measured in the L^2 norm,

$$\chi_{mod}(x,\,t,\,\hbar) \;=\; \frac{P_0(x,E^*)\,\sqrt{2\,\pi\,\hbar}}{\sqrt{\alpha''(E^*)\,+\,i\,S''(x,\,t,\,E^*)}}\;e^{-\,(\alpha(E^*)\,+\,i\,S(x,t,E^*))/\hbar}\;e^{-\,\frac{S'(x,\,t,\,E^*)^2}{2\,\hbar\,(\alpha''(E^*)\,+\,i\,S''(x,\,t,\,E^*))}},$$

and $'$ denotes the derivative with respect to E.

Proof Outline We follow the main steps of the proof of the corresponding result for Theorem 5 of [2], with one notable exception. Since we do not use any superadiabatic representation, the next to leading order term in the asymptotics of $c^a(x,\,E,\,\hbar)$ is of too low an order to be treated as in [2]. We briefly address this issue in more detail. By integration by parts, we see that for $x > 1$,

$$c^a(x,E,\hbar) \;=\; 1 \;+\; i\,\hbar \int_x^{\infty} \frac{\left(\frac{\partial p}{\partial x}(y,\,E)\right)^2}{8\,p^3(y,\,E)}\,dy \;+\; O_E(\hbar^2/x^{\nu+1}).$$

When we integrate against the energy density $Q(E, \hbar)$, the remainder term can be dealt with by using Lemma 1 of [2]. The non-zero next to leading term is only of order $\hbar/x^{\nu+1}$ and the error term it generates can be bounded as follows:

Let $\eta(x, t, \hbar) = \chi(x, t, \hbar) - \widetilde{\chi}(x, t, \hbar)$, where

$$\widetilde{\chi}(x, E, \hbar) \tag{2.21}$$

$$= \frac{e^{-K(E)/(2\hbar)} \sqrt{p(-\infty, E)}\; e^{i\int_{x_1(E)}^{x} p_R(y, E)\, dy/\hbar}}{\sqrt{p(x, E)}\; c_2^b(-\infty, E, \hbar)\; e^{-i\int_{-\infty}^{x_0(E)}(p_R(y,E)-p_R(-\infty,E))/\hbar}\; e^{-i\, p_R(-\infty, E)\, x_0(E)}}.$$

The error term whose L^2 norm we need to bound has the explicit form

$$\begin{aligned} g(x, t, \hbar) &:= i\hbar \int_\Delta Q(E, \hbar)\, e^{-iEt/\hbar}\, \widetilde{\chi}(x, E, \hbar) \int_x^\infty \frac{\left(\frac{\partial p}{\partial x}(y, E)\right)^2}{8\, p^3(y, E)}\, dy\, dE \\ &\equiv \hbar \int_\Delta e^{-iEt/\hbar}\, \widetilde{Q}(E, \hbar)\, f(x, E)\, e^{i\int_{x_1(E)}^{x} p_R(y, E)\, dy/\hbar}\, dE, \end{aligned}$$

where $f(x, E) = O(1/x^{\nu+1})$, uniformly for $E \in \Delta$, $\widetilde{Q}(E, \hbar)$ is independent of x, and $|\widetilde{Q}(E, \hbar)|$ behaves essentially as $e^{-\alpha(E^*)/\hbar}$ times a Gaussian in $(E - E^*)/\sqrt{\hbar}$. (See (2.18)). We compute

$$\int_{x>1} |g(x, t, \hbar)|^2\, dx \tag{2.22}$$

$$= \hbar^2 \int_{\Delta\times\Delta} \widetilde{Q}(E, \hbar)\, \overline{\widetilde{Q}}(E', \hbar) \int_1^\infty f(x, E)\, \overline{f}(x, E')\, e^{i\int_{x_1(E)}^{x}(p_R(y, E)-p_R(y, E'))\, dy/\hbar}\, dx\, dE\, dE'.$$

Let $0 < \theta < 1$. We split the integration range into the sets where $|E - E'| < \hbar^\theta$ and $|E - E'| \geq \hbar^\theta$. We perform an integration by parts in x on the latter set to get

$$\begin{aligned} &\int_1^\infty f(x, E)\, \overline{f}(x, E')\, e^{i\int_{x_1(E)}^{x}(p_R(y, E)-p_R(y, E'))\, dy/\hbar}\, dx \\ &= \frac{i\hbar}{2\,(E - E')}\, (p_R(1, E) + p_R(1, E'))\, f(1, E)\, \overline{f}(1, E')\, e^{i\int_{x_1(E)}^{1}(p_R(y, E)-p_R(y, E'))\, dy/\hbar} \\ &+ \frac{i\hbar}{2(E - E')} \int_1^\infty \frac{\partial}{\partial x}\Big((p_R(x, E) + p_R(x, E'))\, f(x, E)\, \overline{f}(x, E') \Big) \\ &\qquad\qquad \times\; e^{i\int_{x_1(E)}^{x}(p_R(y, E)-p_R(y, E'))\, dy/\hbar}\, dx. \end{aligned}$$

The absolute values of both terms are bounded by $C\hbar^{1-\theta}$, where C is uniform in E. So, they contribute a factor $C\hbar^{3-\theta}\|\widetilde{Q}\|_1^2$ to (2.22). Similarly, the integral in x in (2.22) is bounded uniformly in E and, for some constant C,

$$\int_{\Delta\times\Delta} |\widetilde{Q}(E,\hbar)|\, |\widetilde{Q}(E',\hbar)|\, \chi_{\{|E-E'|<\hbar^\theta\}}\, dE\, dE' \ \leq\ C\, \|\widetilde{Q}\|_2^2\, \hbar^{\theta/2}.$$

Since Δ is compact, $\|\widetilde{Q}\|_1 \leq |\Delta|^{1/2}\|\widetilde{Q}\|_2$. Using this and the the estimate $\|\widetilde{Q}\|_2 \leq Ce^{-\alpha(E^*)/\hbar}\hbar^{1/4}$, we eventually get for $\theta = 2/3$,

$$\|g\|_2 \ \leq\ C\, e^{-\alpha(E^*)/\hbar}\, \hbar^{17/12} \ \ll\ C\, e^{-\alpha(E^*)/\hbar}\, \hbar^{3/4}.$$

The rest of the proof, which consists of showing that $\widetilde{\chi}$ can be approximated by χ_{mod} and χ^{∞}_{Gauss} for different values of x, now relies on Lemma 2.3 and on arguments identical to those in the proof of Theorem 5 of [2]. ■

While explicit and concise, the approximation above does not make apparent where the transmitted wave is actually located. To have a better idea of the position of this wave function, we define q_t to be the unique solution in x to $\dfrac{\partial}{\partial E}\, S(x,\, t,\, E^*) = 0$ with $q_t > 0$ and $\dot{q}_t > 0$. The function q_t is actually the classical trajectory in the potential V with energy E^*, the velocity of which is bounded from above and below. We define

$$\chi_{Gauss}(x,\, t,\, \hbar) \ = \ \frac{P_0(q_t,\, E^*)\, \sqrt{2\,\pi\,\hbar}}{\sqrt{\alpha''(E^*)\, +\, i\, S''(q_t,\, t,\, E^*)}}\ \exp\{-(\alpha(E^*)\, +\, i\, S(x,\, t,\, E^*))/\hbar\}$$

$$\times \quad \exp\left\{-\ \frac{(x\, -\, q_t)^2}{2\,\hbar\, p_R(q_t,\, E^*)^2\, (\alpha''(E^*)\, +\, i\, S''(q_t,\, t,\, E^*))}\right\}.$$

This wave packet is a Gaussian that is centered on the trajectory q_t, and whose width is of order $\sqrt{\hbar}$.

This leads immediately to the following corollary. (See Theorem 6 of [2].)

Corollary 2.6 *There exist* $X_0 > 0$ *and* $\delta > 0$, *such that for all times* t, *with* $X_0 < q_t < C\hbar^{-\beta}$, *we have, in the* L^2 *sense,*

$$\chi(x,\, t,\, \hbar) \ = \ \chi_{Gauss}(x,\, t,\, \hbar) \ +\ O\left(\hbar^{3/4+\delta}\, e^{-\alpha(E^*)/\hbar}\right),$$

where $\quad \|\chi_{Gauss}(x,\, t,\, \hbar)\|_{L^2} \ = \ O\left(\hbar^{3/4}\, e^{-\alpha(E^*)/\hbar}\right).$

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