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The Landau-Zener Problem in the Light of the Stokes Geometry

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Abstract: We show how to derive the transition probabilities in the Landau-Zener effect via the Stokes geometry.

Keywords: Landau-Zener model, Stokes geometry, WKB approximations, asymptotic series, Borel summation

1 Introduction

In complex analysis, the Stokes phenomenon (named after George G. Stokes who discovered it in 1847-1858) is that the asymptotic behaviour of functions can differ in different regions of the complex plane. When second-order linear ordinary differential equations :

$$\hbar^2 \frac{d^2y}{dx^2} + Q(x)y = 0 \tag{1}$$

where $Q(x)$ is an irreducible rational function, are considered, the principal parts of the formal solutions are of the form :

$$y(x,\hbar) \sim \frac{1}{Q(x)^{1/4}} \exp\left(\pm\frac{i}{\hbar}\int^x Q(s)^{1/2} ds\right)$$

which are called WKB approximations. The regions or domains in which the WKB approximations of (1) are valid are determined by the so-called phase-integral :

$$\xi(x,t) = \int_{x_0}^{x} Q(s)^{1/2} ds \tag{2}$$

where x_0 is any of the turning points of (1). Since we must consider two WKB approximations on two sheets of complex planes, it is sufficient for our purpose to choose one of the two square roots of the integrand of the integral (2). Canonical regions around the turning point x_0 are bounded by the level lines $\mathrm{Re}\,\xi(x,t) = 0$ (Stokes lines) and $\mathrm{Im}\,\xi(x,t) = 0$ (anti-Stokes lines). More details about the Stokes phenomenon can be found in [1], [6] or [7] for instance - as well as the multiple references therein. For an in-depth comprehension and beyond, the interested reader should confer to the various works of Robert B. Dingle [4], John Heading [5], and Michael V. Berry [2], [3].

We focus on the Landau-Zener model (see [8] for notations). This paper is divided into five parts :

- as usual, Section 2 concerns some generalities and definitions,
- in Section 3, from the Schrödinger equation for the wave component ψ_1, we extract two series representations that will be crucially required in both Sections 4 and 6,
- by only assuming $z \gg \hbar$ in Section 4, we shall exhibit a geometrical technique to derive the two Landau-Zener transition probabilities :

$$\begin{cases} a_{LZ}(z) = \exp\left(-\frac{\pi z^2}{2\hbar}\right) \\ b_{LZ}(z) = \frac{2i}{z} e^{i\frac{\pi}{4}} \sqrt{\frac{\hbar}{\pi}} \left(\frac{\hbar}{2}\right)^{i\frac{z^2}{2\hbar}} \Gamma\left(1+i\frac{z^2}{2\hbar}\right) \exp\left(-\frac{\pi z^2}{4\hbar}\right) \sinh\frac{\pi z^2}{2\hbar} \end{cases}, \tag{3}$$

  due to the continuation of the WKB approximations through the Stokes diagram, namely once the singularities, the action W and the Stokes constant $C_S\left(\frac{3\pi}{4}\right)$ are known ; while in Section 5, we show the efficiency of the SDE in the diabatic limit too,
- regardless to the accurate expressions of Section 4, the adiabatic limit $0 < z \ll \hbar$ is naively carried out in Section 6, leading thus to a discrepancy that is examined.

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For the S-matrix, we shall make straightforward use of several rules derived in the end of [10]. Note that all the results are remarkably consistent with (3).

2 The Stokes geometry

2.1 Generalities about the WKB analysis

The problem is that the approximate solutions exist in disconnected domains of the real axis, and they must be connected across the intervening domains where they are not valid. For instance, the presence of the factor $\frac{1}{t}$ (before the functions $e^{\pm i\Lambda_p(t,\cdot)}$ in [10]) prevents the prolongation of the approximate solutions through the origin. Analytic continuation in $\mathbb{C}$ provides the means of connection. But although the exact solution to the differential equation may be analytic and thus valid everywhere, the approximate solutions are not and have very different properties from the exact solution, including the existence of cuts.
George Gabriel Stokes was the first to deal with the asymptotic approximations of the Airy equation, realizing in 1857 that discontinuities in the form of the asymptotic representation existed at the so-called Stokes lines, even though the functions themselves are continuous. Lord Rayleigh considered such approximate solutions in 1912, but he did not succeed in making the connection across the gap. More systematic approaches to matching the solutions were obtained by Gregor Wentzel, Hans Kramers and Léon Brillouin in 1926, when the interest was primarily in obtaining solutions to bound state problems in quantum mechanics.
The theory was finally put in form by Harold Jeffreys and John Heading in 1962. It offers a very powerful means of obtaining reasonably good approximate solutions to differential equations, and is often used in electromagnetism, quantum mechanics, and other disciplines.

2.2 Asymptotic solutions

Joseph Liouville and George Green may be said to have founded the method in 1837, and it is also commonly referred to as the Liouville-Green method. The important contribution of Harold Jeffreys, Gregor Wentzel, Hans Kramers and Léon Brillouin to the method was the inclusion of the treatment of turning points, connecting the evanescent and oscillatory solutions at either side of the turning point.
The power and simplicity of phase-integral methods for the approximate solution of differential equations make them a common tool in physics, when the equations are often too cumbersome to solve by standard exact methods. The physical problem is initially defined on the real axis. However, the differential equation is analytically prolonged into the complex plane.
By analogy with physics, we shall call the function $Q(x)$ in (1) the pulsation of the system (or equivalently, its frequence). This quantity is actually related to the refractive index of a medium. The asymptotic theory of (1) has been divided into two cases, depending on whether or not $Q(x)$ has isolated zeroes or singularities (namely poles). If $Q(x)$ does not vanish then (1) falls within the scope of a systematic theory. However, if $Q(x)$ has isolated zeroes or singularities, individual representatives of (1) become peculiar. Such special cases are called ”turning point” problems, and the zeroes or singularities of $Q(x)$ are called ”turning points”.

2.3 Classification of singularities

(Fuchs) Differential equations are classified according to their singularity structure. Let us consider the n-th order linear differential equation :

$$Lf = f^{(n)} + P_{n-1}(x)f^{(n-1)} + \ldots + P_0(x)f = 0\,.$$

Definition 1. *A point x_0 is called an ordinary point if all the $P_k(x)$ are analytic at this point, naturally considered as functions of the complex variable x.*

In this case, the solutions of the differential equation possess Taylor series which converge within a disk with radius at least as large as the distance to the nearest singularity of the P_k.

Definition 2. *A point x_0 is called a regular singular point if the functions $(x-x_0)^n P_0$, $(x-x_0)^{n-1}P_1$, ..., $(x-x_0)P_{n-1}$ are analytic at x_0.*

If a point x_0 is neither an ordinary nor a regular singular point, it is called an irregular (or essential) singular point. In this case, there is no convergent series representation of the solution around this point. Then the solution $f(x)$ has an essential singularity at this point, meaning that neither $\lim_{x\to x_0} f$ nor $\lim_{x\to x_0} \frac{1}{f}$ exists. The Picard theorem states that in any neighbourhood $\mathscr{U}_{x_0}$ of an essential singularity, f takes on every complex value, except possibly one. Nevertheless, it is often possible to find local asymptotic series which approach the solution to within some small error and thereafter diverge.

Definition 3(Darboux principle). *One may derive an asymptotic expansion in degree j for the coefficients a_j of a series solely from knowledge of the singularities of the function $f(x)$ that the series represents. This principle applies to any power series and divergent power series.*

Definition 4. *Turning points (or equivalently, transition points) are certain exceptional values of x for analytic differential systems of the type (1).*

Stated differently : in a neighbourhood of such points, the functional character of the solution undergoes substantial metamorphosis. At a transition point :

trigonometric solutions $\leftarrow$ $f(x)$ $\rightarrow$ exponential solutions

neutral behaviour $\leftarrow$ functional character $\rightarrow$ subdominant or dominant behaviour .

(Poincaré) Provided that $\left|\frac{1}{Q^{3/2}}\frac{dQ}{dx}\right| \ll 1$, and setting :

$$y_{\pm}(x) = \frac{1}{Q(x)^{1/4}} \exp\left(\pm\frac{i}{\hbar}\int^{x} Q(s)^{1/2} ds\right) ,$$

a general solution of (1) can then be approximated by a linear combination $y(x) = c_+ y_+(x) + c_- y_-(x)$. Unfortunately, the approximate solutions $y_{\pm}$ are local, not global solutions, and clearly not valid in the vicinity of a zero of $Q(x)$. The phase-integral method consists in relating for a given solution of (1), the WKB approximation in one region of the complex plane to that in another. These (canonical) regions are separated by the Stokes and anti-Stokes lines associated with $Q(x)$ - or more generally by these level surfaces of codimension 1 when one works in $\mathbb{C}^n$. Thus the qualitative properties of the solution are determined once these lines are known.

Definition 5. *The Stokes (respectively anti-Stokes) lines associated to $Q(x)$ are paths in the complex plane, emanating from zeroes or singularities x_0 of $Q(x)$, along which $\int_{x_0} Q(s)^{1/2} ds$ is imaginary (respectively real).*

Along the anti-Stokes lines, the functions $y_{\pm}$ are, within the validity of the WKB approximation, of constant amplitude i.e. oscillatory : they are said neutral and that is why the subscripts s or d are sometimes dropped. Similarly along the Stokes lines, the WKB solutions are exponentially increasing or decreasing with fixed phase. The global anti-Stokes and Stokes lines which are attached to the singularities of the differential equation in the Stokes diagram, along with the Riemann cut lines, determine the global properties of the WKB solutions.
In the notation of Heading, a local WKB approximate solution is denoted by :

$$(a,x)_s = \frac{1}{Q^{1/4}} \exp\left(\frac{i}{\hbar}\int_a^x Q(s)^{1/2} ds\right) , \qquad (4)$$

where the subscript s (or d) indicates that the solution is subdominant (or dominant), i.e. exponentially decreasing (or increasing) for increasing $|x-a|$ in a particular region of the x plane, bounded by Stokes and anti-Stokes lines. The two independent local WKB approximate solutions of (1) are given by $(a,x)_s$ and $(x,a)_d$. Of course when one function is dominant, then the other one is subdominant.

2.4 Connection formulae

In a domain far from any zero or singularity of $Q(x)$, the solution to the differential equation in WKB approximation is simply given by the eikonal representation (4).
(Jeffreys, Heading) Denote by x a generic point in $\mathbb{C}$. Begin with a particular solution in one region of the complex plane, choosing that combination of subdominant and dominant solutions which gives the desired boundary conditions in this region. The global solution is obtained by continuing this solution through the whole complex plane, effecting the following changes :

- upon crossing a cut in a counterclockwise sense, the cut originating for a first-order zero of Q at the point a :

$$(a,x)_\bullet \longrightarrow -i(x,a)_\bullet$$
$$(x,a)_\bullet \longrightarrow -i(a,x)_\bullet ,$$

  and the property of dominancy or subdominancy is preserved in the process
- upon crossing an anti-Stokes line, subdominant solutions become dominant, and vice versa
- upon crossing a Stokes line in a counterclockwise sense, the coefficient α_s of the subdominant term of a solution must be replaced by $\alpha_s + C_S\alpha_d$, where C_S is called the Stokes constant
- reconnect from singularity a to singularity b, using :

$$(x,a)_\bullet = (x,b)_\bullet [b,a]$$

  with $[b,a] = \exp\left(\frac{i}{\hbar}\int_b^a Q(s)^{1/2} ds\right)$. If a and b are joined by a Stokes line, reconnect while on the line, using $1/2$ the usual Stokes constant to step on the line, again $1/2$ to step off.

Using the so-called connection formulae, we can pass from region to region across the cuts, anti-Stokes and Stokes lines emanating from a turning point. Beginning with any combination of dominant and subdominant WKB solutions in one region, this process leads to a globally defined single-valued approximate solution of (1). At a Stokes line in the presence of a dominant solution, the apparent ”discontinuity” produced is small in comparison to the error due to the WKB approximation itself. As one continues further away from the Stokes line, however, the subdominant term will begin to be important, and the modified coefficient is the correct one. Note that a Stokes structure consisting of multiple singularities is more complicated, in the sense that the Stokes constants tied to a turning point are modified by the proximity of the other singularities.

3 Construction of the asymptotic series for the Landau-Zener problem

From [8], we know that the second-order linear ODE :

$$\hbar^2\frac{d^2\psi_1}{dt^2}+(t^2+z^2-i\hbar)\psi_1=0 \qquad (5)$$

is a partial reformulation of the Landau-Zener model. Solutions of (5) have an essential singularity at infinity. The WKB approximations of (5) involve two exponentials $\exp\left(\pm\frac{it^2}{2\hbar}\right)$, both affected by the Stokes phenomenon. At some point, we might need to determine the Stokes constant in the direction $\operatorname{Arg} t=\frac{3\pi}{4}$. After extracting the asymptotic behaviour $\psi_1(t)=f(t)\exp\left(-\frac{it^2}{2\hbar}\right)$, we are looking for a power series representation of the function f. By Liebniz formula :

$$\frac{d^2\psi_1}{dt^2}=\left[f''-\frac{2it}{\hbar}f'+\left(-\frac{i}{\hbar}-\frac{t^2}{\hbar^2}\right)f\right]\exp\left(-\frac{it^2}{2\hbar}\right).$$

Inserting this expression into (5), we get :

$$f''-\frac{2it}{\hbar}f'+\left(\frac{z^2}{\hbar^2}-\frac{2i}{\hbar}\right)f=0\,.$$

For convenience, we shall make an extensive use of the (decreasing) Pochhammer symbol $(x)_{(n)}$ defined by :

$$\begin{aligned}\forall n\in\mathbb{N},\ (x)_{(n)}&=x(x-1)\dots(x-n+1)\\&=\frac{\Gamma(x+1)}{\Gamma(x-n+1)}\,,\end{aligned} \qquad (6)$$

with the convention $(x)_{(0)}=1$. Since there is no misunderstanding possible throughout this paper, we will denote it simply by x_n in order to lighten notations. This falling sequential product is sometimes called the descending factorial. Now write $f(t)=t^\nu\sum_{k=0}^{+\infty}c_kt^k$, yielding :

$$f'(t)=t^{\nu-1}\sum_{k=0}^{+\infty}(\nu+k)c_kt^k\,,\ f''(t)=t^{\nu-2}\sum_{k=0}^{+\infty}(\nu+k)_2c_kt^k\,.$$

The second-order ODE defining f becomes :

$$\begin{aligned}&\frac{1}{t^2}\sum_{k=0}^{+\infty}(\nu+k)_2c_kt^k-\frac{2i}{\hbar}\sum_{k=0}^{+\infty}(\nu+k)c_kt^k+\left(\frac{z^2}{\hbar^2}-\frac{2i}{\hbar}\right)\sum_{k=0}^{+\infty}c_kt^k=0\\ \Longleftrightarrow\ &\frac{1}{t^2}\sum_{k=0}^{+\infty}(\nu+k)_2c_kt^k+\sum_{k=0}^{+\infty}\left[\frac{z^2}{\hbar^2}-\frac{2i(\nu+k+1)}{\hbar}\right]c_kt^k=0\,.\end{aligned}$$

The indicial equation gives the necessary condition $\nu(\nu-1)=0$. That implies $\nu\in\{0,1\}$. When choosing $\nu=0$, a quick inspection shows that every odd index coefficients vanish as c_1 can be arbitrary set to 0. For the order $2(k-1)$, from the recurrence relation :

$$(\nu+2k)_2c_{2k}+\left[\frac{z^2}{\hbar^2}-\frac{2i\left[\nu+2(k-1)+1\right]}{\hbar}\right]c_{2(k-1)}=0\,,$$

we thus get :

$$\begin{aligned}\forall k\geqslant 1,\ c_{2k}&=\frac{1}{(\nu+2k)_2}\left[\frac{2i\left[\nu+2(k-1)+1\right]}{\hbar}-\frac{z^2}{\hbar^2}\right]c_{2(k-1)}\\&=\frac{1}{(\nu+2k)!}\prod_{\ell=0}^{k-1}\left[\frac{2i(\nu+2\ell+1)}{\hbar}-\frac{z^2}{\hbar^2}\right]\,.\end{aligned} \qquad (7)$$

Thus, the general power series solution is :

$$\begin{aligned}f(t)=&\ A\underbrace{\left(1+\sum_{k=1}^{+\infty}\frac{1}{(2k)!}\prod_{\ell=0}^{k-1}\left[\frac{2i(2\ell+1)}{\hbar}-\frac{z^2}{\hbar^2}\right]t^{2k}\right)}_{f_1(t)}\\&+B\underbrace{\left(1+\sum_{k=1}^{+\infty}\frac{1}{(2k+1)!}\prod_{\ell=1}^{k}\left[\frac{2i(2\ell)}{\hbar}-\frac{z^2}{\hbar^2}\right]t^{2k}\right)t}_{f_2(t)}\end{aligned}$$

and $\psi_1(t,z)=\left[Af_1(t)+Bf_2(t)\right]\exp\left(-\frac{it^2}{2\hbar}\right)$

as a linear combination of two independent functions. On the other hand, if we make the substitution $\psi_1=g(t)\exp\left(\frac{it^2}{2\hbar}\right)$ instead of $f(t)\exp\left(-\frac{it^2}{2\hbar}\right)$ in (5) :

$$g''+\frac{2it}{\hbar}g'+\frac{z^2}{\hbar^2}g=0\,.$$

Put $g(t)=t^\nu\sum_{k=0}^{+\infty}d_kt^k$ with $d_0=1$, and we obtain :

$$\begin{aligned}&\frac{1}{t^2}\sum_{k=0}^{+\infty}(\nu+k)_2d_kt^k+\frac{2i}{\hbar}\sum_{k=0}^{+\infty}(\nu+k)d_kt^k+\frac{z^2}{\hbar^2}\sum_{k=0}^{+\infty}d_kt^k=0\\ \Longleftrightarrow\ &\frac{1}{t^2}\sum_{k=0}^{+\infty}(\nu+k)_2d_kt^k+\sum_{k=0}^{+\infty}\left[\frac{2i(\nu+k)}{\hbar}+\frac{z^2}{\hbar^2}\right]d_kt^k=0\,.\end{aligned}$$

As before, $\nu\in\{0,1\}$. And in the same way, we get :

$$\forall k\geqslant 1,\ d_{2k}=\frac{(-1)^k}{(\nu+2k)!}\prod_{\ell=0}^{k-1}\left[\frac{2i(\nu+2\ell)}{\hbar}+\frac{z^2}{\hbar^2}\right]\,. \qquad (8)$$

So the general power series solution is now :

$$\begin{aligned}g(t)=&\ A\underbrace{\left(1-\frac{z^2}{2\hbar^2}t^2+\sum_{k=2}^{+\infty}\frac{(-1)^k}{(2k)!}\frac{z^2}{\hbar^2}\prod_{\ell=1}^{k-1}\left[\frac{2i(2\ell)}{\hbar}+\frac{z^2}{\hbar^2}\right]t^{2k}\right)}_{g_1(t)}\\&+B\underbrace{\left(1+\sum_{k=1}^{+\infty}\frac{(-1)^k}{(2k+1)!}\prod_{\ell=0}^{k-1}\left[\frac{2i(2\ell+1)}{\hbar}+\frac{z^2}{\hbar^2}\right]t^{2k}\right)t}_{g_2(t)}\end{aligned}$$

and $\psi_1(t,z)=\left[Ag_1(t)+Bg_2(t)\right]\exp\left(\frac{it^2}{2\hbar}\right)$

The series $\sum_{k=0}^{+\infty} c_k t^{k+\nu}$ is an example of asymptotic series. This definition includes the cases of series which converge, either for all t or for a restricted range of t, but normally when one refers to an asymptotic series, it is understood that the series in question is divergent. The study of asymptotic series was first made by Henri Poincaré. A series $\sum_{n=0}^{+\infty} a_n x^n$ is said to be asymptotic to a function $f(x)$ at $x=0$, or $f(x) \underset{0}{\sim} \sum_{n=0}^{+\infty} a_n x^n$, if for $x \to 0$, we have :

$$f(x) - \sum_{n=0}^{N} a_n x^n \ll x^N \quad \text{for all } N \, .$$

If an asymptotic expansion of a function f exists, then the coefficients a_n are unique, and given by the limiting procedure :

$$a_0 = \lim_{x\to 0} f(x) \quad , \quad a_1 = \lim_{x\to 0} \frac{f(x)-a_0}{x} \quad , \quad \text{etc .}$$

The converse is false : indeed to $f(x)$, one can add any function which decreases faster than any power of x without changing the asymptotic expansion. The class of all functions which are asymptotically equal to f is defined as the sum of the asymptotic series.

Remark 1*If the series diverges, this can be an indication that the function is not analytic at the point of the expansion, and not that the function is infinite or otherwise ill-defined.*

A means of summing divergent series is the Borel summation. This powerful technique often extends the domain in which the sum "converges" beyond the normal radius of convergence.

4 Revisiting Landau-Zener, part 1 : when $z \gg \hbar$

In this section, we assume that $\hbar$ is small before the coupling parameter z. Recall (5) :

$$\hbar^2 \frac{d^2\psi_1}{dt^2} + (t^2 + z^2 - i\hbar)\psi_1 = 0 \, .$$

There will be repercussions in the structure of the Stokes diagram, and the action W between the turning points.

4.1 Stokes diagram

Here since $z \gg \hbar$, the pulsation $Q(t,z) = t^2 + z^2 - i\hbar$ is almost real and positive on the real axis, with two simple

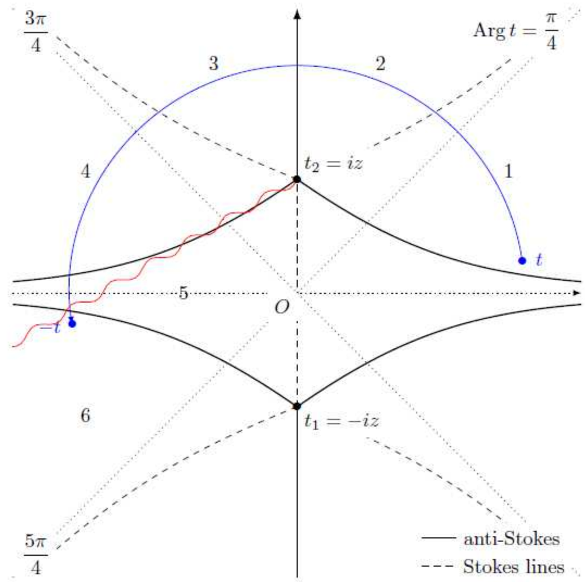

Fig. 1: Stokes structure for 2 simple turning points on the imaginary axis.

zeroes close to $\pm iz$. Hence the resulting diagram (where some distances were exaggerated for clarity) :
In the Stokes diagram, we deliberately begin with a subdominant solution so that the solution is small and cannot contain any dominant part due to the approximate nature of the WKB solution. Continuation through the upper half-plane gives :

1.start on the positive real axis with the subdominant solution : $(iz,t)_s$
2.crossing a Stokes line : $(iz,t)_s$
3.crossing an anti-Stokes line : $(iz,t)_d$
4.crossing a Stokes line : $(iz,t)_d + C_S(t,iz)_s$
5.crossing an anti-Stokes line : $(iz,t)_s + C_S(t,iz)_d$
reconnecting iz to $-iz$ on the left of the cut :
$[iz,-iz]_\ell(-iz,t)_s + C_S(t,-iz)_d[-iz,iz]_\ell$
6.passing the cut in a counterclockwise sense :
$[iz,-iz]_\ell(t,-iz)_s + C_S(-iz,t)_d[-iz,iz]_\ell$
as reaching the negative axis, rename t into $-t$:
$[iz,-iz]_\ell(-t,-iz)_s + C_S(-iz,-t)_d[-iz,iz]_\ell$

where C_S is the Stokes constant associated with the zero at $t_2 = iz$ and the direction $\text{Arg}\, t = \frac{3\pi}{4}$. Subscripts ℓ and r stand for "left" and "right" of the cut. Let us compute the quantity :

$$W = -\frac{i}{\hbar}\int_{-iz}^{iz} \sqrt{t^2+z^2}\, dt = \frac{\pi z^2}{2\hbar}$$

which is called the (left) action from the turning point $t_1 = -iz$ to $t_2 = iz$. Note that W is proportional to the Wallis integral $I_2 = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \cos^2\theta\, d\theta$. The factor $[-iz,iz]_\ell$

turns out to be equal to e^W. Consequently, for a subdominant solution in domain 1 :

$$\psi_1(t) = (iz,t)_s$$

i.e. with the correction $\exp S_1^+(+\infty) = 1$, we end up in domain 6 with :

$$\psi_1(-t) = e^{-W}(-iz,-t)_s + C_S e^W(-t,-iz)_d$$

as $t \to +\infty$. Take the reference point for the phase to be $\tau = 0$. Formally divide both sides by $[iz,0]_r$, then :

$$e^{-W}(0,-t)_s + C_S e^W(-t,0)_d \quad \leftrightsquigarrow \quad (0,t)_s \qquad (9)$$

since $[iz,0]_r[0,-iz]_\ell = 1$. This may be the shortest proof ever of $a(z) = \exp\left(-\frac{\pi z^2}{2\hbar}\right)$.

4.2 Dominant exponential solutions in the $\frac{k\pi}{4}$ directions

Lemma 1. *For $\alpha \in \mathbb{C}$ fixed. For $x \in \mathbb{C}$ such that $\mathrm{Re}\,x > 0$, one has :*

$$\frac{\Gamma(x)}{\Gamma(x+\alpha)} = \frac{1}{x^\alpha} + \mathscr{O}\left(\frac{1}{|x|^{1+\mathrm{Re}\,\alpha}}\right)$$

as $|x| \to +\infty$.

Proof. It is essentially based on Watson's lemma. Start with the Beta function defined as :

$$B(x,\alpha) = \frac{\Gamma(x)\Gamma(\alpha)}{\Gamma(x+\alpha)} = \int_0^1 t^{x-1}(1-t)^{\alpha-1}dt\ .$$

Fix α with $\mathrm{Re}\,\alpha > 0$, and consider this integral as a function of x. Letting $t = e^{-u}$ yields :

$$\begin{aligned} B(x,\alpha) &= \int_0^{+\infty} e^{-xu}\left(1-e^{-u}\right)^{\alpha-1} du \\ &= \int_0^{+\infty} e^{-xu}u^{\alpha-1}\left(1-\frac{u}{2!}+\dots\right)^{\alpha-1} du \simeq \frac{\Gamma(\alpha)}{x^\alpha} \end{aligned}$$

by only taking the first term in the expansion when $\mathrm{Re}\,x > 0$, and thus the error is bounded by a $\mathscr{O}\left(\frac{1}{|x|^{1+\mathrm{Re}\,\alpha}}\right)$ term. Dividing both sides by $\Gamma(\alpha)$ gives the desired result. ■

From (7), the general term of f_1 is :

$$\begin{aligned} c_{2n}t^{2n} &= \frac{1}{(2n)!}\prod_{\ell=0}^{n-1}\left[\frac{2i(2\ell+1)}{\hbar} - \frac{z^2}{\hbar^2}\right]t^{2n} \\ &= \frac{2^n}{(2n)!}\left(\frac{2i}{\hbar}\right)^n \prod_{\ell=0}^{n-1}\left(\ell+\frac{1}{2}+\frac{iz^2}{4\hbar}\right)t^{2n} \\ &= \frac{2^n}{(2n)!}\left(\frac{2i}{\hbar}\right)^n \left(n-\frac{1}{2}+\frac{iz^2}{4\hbar}\right)_n t^{2n} \\ &= \frac{2^n}{(2n)!}\left(\frac{2i}{\hbar}\right)^n \frac{\Gamma\left(n+\frac{1}{2}+i\frac{z^2}{4\hbar}\right)}{\Gamma\left(\frac{1}{2}+i\frac{z^2}{4\hbar}\right)} t^{2n}\ . \end{aligned}$$

Let us now determine the asymptotic expressions of ψ_1 on the Stokes lines $\mathrm{Arg}\,t = -\frac{\pi}{4}$ or $\mathrm{Arg}\,t = \frac{3\pi}{4}$.

When $t = Te^{-i\frac{\pi}{4}}$ or $Te^{i\frac{3\pi}{4}}$ - with T real, large and positive (in a sense, we might think of T as $+\infty$), we have :

$$\begin{aligned} f_1(t) &= \sum_{n=0}^{+\infty}\left(\frac{4}{\hbar}\right)^n \frac{\Gamma\left(n+\frac{1}{2}+i\frac{z^2}{4\hbar}\right)}{\Gamma\left(\frac{1}{2}+i\frac{z^2}{4\hbar}\right)}\frac{T^{2n}}{(2n)!} \\ &\simeq \sum_{n=0}^{+\infty}\left(\frac{4}{\hbar}\right)^n \frac{n^{-\frac{1}{2}+i\frac{z^2}{4\hbar}}}{\Gamma\left(\frac{1}{2}+i\frac{z^2}{4\hbar}\right)}\sqrt{2\pi n}\left(\frac{n}{e}\right)^n \frac{1}{\sqrt{4\pi n}}\left(\frac{e}{2n}\right)^{2n} T^{2n} \\ &= \sum_{n=0}^{+\infty}\left(\frac{1}{\hbar}\right)^n \frac{n^{-\frac{1}{2}+i\frac{z^2}{4\hbar}}}{\Gamma\left(\frac{1}{2}+i\frac{z^2}{4\hbar}\right)}\frac{1}{\sqrt{2}}\left(\frac{e}{n}\right)^n T^{2n}\ , \end{aligned}$$

by using $\Gamma(n+\delta) \simeq n^\delta\Gamma(n)$ and the Stirling formula $\Gamma(n) \simeq \sqrt{\frac{2\pi}{n}}\left(\frac{n}{e}\right)^n$. We replace these discrete terms by a continuous function, but since a complex index occurs for n, the summands are not wholly real. The factor $n^{-\frac{1}{2}+i\frac{z^2}{4\hbar}}$ is a slowly varying function, compared with the other variable factors. Hence :

$$f_1(t) \simeq \frac{x_0^{-\frac{1}{2}+i\frac{z^2}{4\hbar}}}{\sqrt{2}\Gamma\left(\frac{1}{2}+i\frac{z^2}{4\hbar}\right)}\int_0^{+\infty}\exp\left(x - x\log x + x\log\frac{T^2}{\hbar}\right)dx\ ,$$

with a constant $x_0 \in \mathbb{R}_+$ soon to be determined. The integral is now evaluated by the method of the steepest descent. So if we set $\varphi(x) = x - x\log x + x\log\frac{T^2}{\hbar}$, then :

$$\varphi'(x) = -\log x + \log\frac{T^2}{\hbar} \quad , \quad \varphi''(x) = -\frac{1}{x}\ .$$

Thus $\varphi'(x) = 0$ when $x_0 = \frac{T^2}{\hbar}$, and :

$$\begin{aligned} f_1(t) &\simeq \frac{1}{\sqrt{2}\Gamma\left(\frac{1}{2}+i\frac{z^2}{4\hbar}\right)}\left(\frac{T^2}{\hbar}\right)^{-\frac{1}{2}+i\frac{z^2}{4\hbar}}\sqrt{\frac{2\pi T^2}{\hbar}}\exp\left(\frac{T^2}{\hbar}\right) \\ &= \frac{\sqrt{\pi}}{\Gamma\left(\frac{1}{2}+i\frac{z^2}{4\hbar}\right)}\left(\frac{T^2}{\hbar}\right)^{i\frac{z^2}{4\hbar}}\exp\left(\frac{T^2}{\hbar}\right) \\ &= \frac{\sqrt{\pi}}{\Gamma\left(\frac{1}{2}+i\frac{z^2}{4\hbar}\right)}\left(\frac{it^2}{\hbar}\right)^{i\frac{z^2}{4\hbar}}\exp\left(\frac{it^2}{\hbar}\right) \end{aligned}$$

$$\Longrightarrow \quad \psi_1(t) = f_1(t)\exp\left(-\frac{it^2}{2\hbar}\right) = \frac{\sqrt{\pi}}{\Gamma\left(\frac{1}{2}+i\frac{z^2}{4\hbar}\right)}\left(\frac{it^2}{\hbar}\right)^{i\frac{z^2}{4\hbar}}\exp\left(\frac{it^2}{2\hbar}\right)$$

in the directions $\mathrm{Arg}\,t = -\frac{\pi}{4}$ or $\frac{3\pi}{4}$, and this is indeed a dominant expression due to its $\mathscr{O}\left[\exp\left(\frac{T^2}{2}\right)\right]$ growth.

When $t = Te^{-i\frac{3\pi}{4}}$ or $Te^{i\frac{\pi}{4}}$, we must use the series g_1 instead of f_1 since the latter series would contain alternating signs, but g_1 now has similar signs throughout. From (8), the general term of g_1 is :

$$d_{2n}t^{2n} = \frac{(-1)^n}{(2n)!}\prod_{\ell=0}^{n-1}\left(\frac{4i\ell}{\hbar}+\frac{z^2}{\hbar^2}\right)t^{2n}$$
$$= \frac{1}{(2n)!}\left(-\frac{4i}{\hbar}\right)^n\left(-\frac{iz^2}{4\hbar}\right)\frac{\Gamma\left(n-i\frac{z^2}{4\hbar}\right)}{\Gamma\left(1-i\frac{z^2}{4\hbar}\right)}t^{2n}\,.$$

Therefore :

$$g_1(t) \simeq -\frac{iz^2}{4\hbar}\frac{x_0^{-1-i\frac{z^2}{4\hbar}}}{\sqrt{2}\Gamma\left(1-i\frac{z^2}{4\hbar}\right)}\int_0^{+\infty}\exp\left(x-x\log x+x\log\frac{T^2}{\hbar}\right)dx$$
$$= -\frac{iz^2}{4\hbar}\frac{\sqrt{\pi}}{\Gamma\left(1-i\frac{z^2}{4\hbar}\right)}\left(\frac{T^2}{\hbar}\right)^{-\frac{1}{2}-i\frac{z^2}{4\hbar}}\exp\left(\frac{T^2}{\hbar}\right)$$
$$= -\frac{iz^2}{4\hbar}\frac{\sqrt{\pi}}{\Gamma\left(1-i\frac{z^2}{4\hbar}\right)}\left(-\frac{it^2}{\hbar}\right)^{-\frac{1}{2}-i\frac{z^2}{4\hbar}}\exp\left(-\frac{it^2}{\hbar}\right)$$
$$\Longrightarrow\ \psi_1(t) = g_1(t)\exp\left(\frac{it^2}{2\hbar}\right)$$
$$= -\frac{iz^2}{4\hbar}\frac{\sqrt{\pi}}{\Gamma\left(1-i\frac{z^2}{4\hbar}\right)}\left(-\frac{it^2}{\hbar}\right)^{-\frac{1}{2}-i\frac{z^2}{4\hbar}}\exp\left(-\frac{it^2}{2\hbar}\right)$$

in the directions $\mathrm{Arg}\,t = -\frac{3\pi}{4}$ or $\frac{\pi}{4}$. The Stokes constants may now be calculated.

4.3 Stokes constants and transition probabilities

We have obtained the following asymptotic expressions :

- for $\mathrm{Arg}\,t = -\frac{3\pi}{4}$:

$$\psi_1(t) = -\frac{iz^2}{4\hbar}\frac{\sqrt{\pi}}{\Gamma\left(1-i\frac{z^2}{4\hbar}\right)}\frac{1}{t}\left(-\frac{i}{\hbar}\right)^{-\frac{1}{2}-i\frac{z^2}{4\hbar}}t^{-i\frac{z^2}{2\hbar}}\exp\left(-\frac{it^2}{2\hbar}\right)$$

- for $\mathrm{Arg}\,t = -\frac{\pi}{4}$:

$$\psi_1(t) = \frac{\sqrt{\pi}}{\Gamma\left(\frac{1}{2}+i\frac{z^2}{4\hbar}\right)}\left(\frac{i}{\hbar}\right)^{i\frac{z^2}{4\hbar}}t^{i\frac{z^2}{2\hbar}}\exp\left(\frac{it^2}{2\hbar}\right)$$

- for $\mathrm{Arg}\,t = \frac{\pi}{4}$:

$$\psi_1(t) = -\frac{iz^2}{4\hbar}\frac{\sqrt{\pi}}{\Gamma\left(1-i\frac{z^2}{4\hbar}\right)}\frac{1}{t}\left(-\frac{i}{\hbar}\right)^{-\frac{1}{2}-i\frac{z^2}{4\hbar}}t^{-i\frac{z^2}{2\hbar}}\exp\left(-\frac{it^2}{2\hbar}\right)$$

- for $\mathrm{Arg}\,t = \frac{3\pi}{4}$:

$$\psi_1(t) = \frac{\sqrt{\pi}}{\Gamma\left(\frac{1}{2}+i\frac{z^2}{4\hbar}\right)}\left(\frac{i}{\hbar}\right)^{i\frac{z^2}{4\hbar}}t^{i\frac{z^2}{2\hbar}}\exp\left(\frac{it^2}{2\hbar}\right)\,.$$

Suppose that we are interested in the computation of the Stokes multiplier on a Stokes line at $\mathrm{Arg}\,t = \theta$. If $C_S(\theta)$ denotes the associated Stokes constant, we have :

$$\begin{aligned}&\text{subdominant coefficient at } \theta^+\\ &\quad= \text{subdominant coefficient at } \theta^-\\ &\qquad+ C_S(\theta)\ \text{dominant coefficient at } \theta\,. \end{aligned} \quad (10)$$

In our case, that can be exactly reformulated in terms of dominant coefficients as :

$$\begin{aligned}&\text{dominant coefficient at } \left(\theta+\frac{\pi}{2}\right)^-\\ &\quad= \text{dominant coefficient at } \left(\theta-\frac{\pi}{2}\right)^+\\ &\qquad+ C_S(\theta)\ \text{dominant coefficient at } \theta\,,\end{aligned}$$

yielding the formula :

$$C_S(\theta) = \frac{D\left(\theta+\frac{\pi}{2}\right)-D\left(\theta-\frac{\pi}{2}\right)}{D(\theta)}$$

where the letter D stands as a shorcut for ”dominant coefficient at”. Apply this formula to our situation :

$$C_S\left(\frac{3\pi}{4}\right) = \frac{D\left(\frac{5\pi}{4}\right)-D\left(\frac{\pi}{4}\right)}{D\left(\frac{3\pi}{4}\right)}$$
$$= -\frac{iz^2}{4\hbar}\frac{\Gamma\left(\frac{1}{2}+i\frac{z^2}{4\hbar}\right)}{\Gamma\left(1-i\frac{z^2}{4\hbar}\right)}\frac{1}{t}\left(\frac{1}{\hbar}\right)^{-\frac{1}{2}-i\frac{z^2}{2\hbar}}\frac{\left(e^{-i\frac{5\pi}{4}}\right)^{-1-i\frac{z^2}{2\hbar}}-\left(e^{-i\frac{\pi}{4}}\right)^{-1-i\frac{z^2}{2\hbar}}}{\left(e^{-i\frac{3\pi}{4}}\right)^{i\frac{z^2}{2\hbar}}}$$
$$= \frac{\Gamma\left(\frac{1}{2}+i\frac{z^2}{4\hbar}\right)}{\Gamma\left(-i\frac{z^2}{4\hbar}\right)}\frac{1}{t}\left(\frac{1}{\hbar}\right)^{-\frac{1}{2}-i\frac{z^2}{2\hbar}}\frac{e^{i\frac{5\pi}{4}}\exp\left(-\frac{5\pi z^2}{8\hbar}\right)-e^{i\frac{\pi}{4}}\exp\left(-\frac{\pi z^2}{8\hbar}\right)}{\exp\left(\frac{3\pi z^2}{8\hbar}\right)}$$
$$= -\frac{2ie^{i\frac{\pi}{4}}}{\pi}\sinh\frac{\pi z^2}{4\hbar}\Gamma\left(\frac{1}{2}+i\frac{z^2}{4\hbar}\right)\Gamma\left(1+i\frac{z^2}{4\hbar}\right)\left(\frac{1}{\hbar}\right)^{-\frac{1}{2}-i\frac{z^2}{2\hbar}}\frac{1}{t}\cosh\frac{\pi z^2}{4\hbar}\exp\left(-\frac{3\pi z^2}{4\hbar}\right)$$

by using the reflection relation $\Gamma(\zeta)\Gamma(1-\zeta) = \frac{\pi}{\sin\pi\zeta}$. Further simplifications occur if we use the duplication formula $\Gamma(\zeta)\Gamma\left(\frac{1}{2}+\zeta\right) = \frac{\sqrt{\pi}\Gamma(2\zeta)}{2^{2\zeta-1}}$, yielding :

$$C_S\left(\frac{3\pi}{4}\right) = -ie^{i\frac{\pi}{4}}\sqrt{\frac{\hbar}{\pi}}\sinh\frac{\pi z^2}{2\hbar}\Gamma\left(1+i\frac{z^2}{2\hbar}\right)\left(\frac{\hbar}{2}\right)^{i\frac{z^2}{2\hbar}}\frac{1}{t}\exp\left(-\frac{3\pi z^2}{4\hbar}\right)\,.$$

Thus, by applying Rule 1 of [10] :

$$\begin{aligned}b_{\text{Stokes}}(z) &= \left(-\frac{2}{z}\right)C_S\left(\frac{3\pi}{4}\right)e^W\\ &= \frac{2i}{z}e^{i\frac{\pi}{4}}\sqrt{\frac{\hbar}{\pi}}\left(\frac{\hbar}{2}\right)^{i\frac{z^2}{2\hbar}}\Gamma\left(1+i\frac{z^2}{2\hbar}\right)\exp\left(-\frac{\pi z^2}{4\hbar}\right)\sinh\frac{\pi z^2}{2\hbar}\,,\end{aligned} \quad (11)$$

in plain agreement with the Landau-Zener formula. Subsequently, the transition probabilities are intrinsically related to the continuation of the WKB approximations of (5), bringing into play connection formulae and Stokes constants - or equivalently Stokes matrices.

5 The SDE alternative when $z \gg \hbar$

In this section, we intent to recover an approximation of (11) in the SDE context :

$$\hbar^2 \frac{d^2\phi}{dt^2} + (t^2+z^2)\phi = 0\,. \tag{12}$$

Placing $\phi(t) = f(t)\exp\left(-\frac{it^2}{2\hbar}\right)$, one obtains the linear differential equation :

$$f'' - \frac{2it}{\hbar} f' - \left(\frac{i}{\hbar} - \frac{z^2}{\hbar^2}\right) f = 0\,.$$

Expand $f(t) = t^\nu \sum_{k=0}^{+\infty} c_k t^k$, with the normalization $c_0 = 1$. Then :

$$\forall k \geqslant 1,\; c_{2k} = \frac{1}{(\nu+2k)_{2k}} \prod_{\ell=1}^{k} \left[\frac{i(2\nu+4\ell-3)}{\hbar} - \frac{z^2}{\hbar^2}\right]\,.$$

Likewise :

$$\forall k \geqslant 1,\; d_{2k} = \frac{(-1)^k}{(\nu+2k)_{2k}} \prod_{\ell=1}^{k} \left[\frac{i(2\nu+4\ell-3)}{\hbar} + \frac{z^2}{\hbar^2}\right]\,,$$

by observing that the coefficients d_k can be readily obtained from c_k by complex conjugation.

5.1 Dominant exponential solutions in the $\frac{k\pi}{4}$ directions

Choose $\nu = 0$. Let us now determine the asymptotic expressions on each Stokes line for $\phi(t) = f_1(t)\exp\left(-\frac{it^2}{2\hbar}\right) = g_1(t)\exp\left(\frac{it^2}{2\hbar}\right)$. When $t = Te^{-i\frac{\pi}{4}}$ or $Te^{i\frac{3\pi}{4}}$, the general term $c_{2n}T^{2n}$ is :

$$c_{2n}T^{2n} = \left(\frac{4}{\hbar}\right)^n \frac{\Gamma\left(n+\frac{1}{4}+i\frac{z^2}{4\hbar}\right)}{\Gamma\left(\frac{1}{4}+i\frac{z^2}{4\hbar}\right)} \frac{T^{2n}}{(2n)!}$$
$$\simeq \left(\frac{1}{\hbar}\right)^n \frac{n^{-\frac{3}{4}+i\frac{z^2}{4\hbar}}}{\sqrt{2}\Gamma\left(\frac{1}{4}+i\frac{z^2}{4\hbar}\right)} \left(\frac{e}{n}\right)^n T^{2n}\,.$$

So :

$$f_1(t) = \frac{\sqrt{\pi}}{\Gamma\left(\frac{1}{4}+i\frac{z^2}{4\hbar}\right)} \left(\frac{i}{\hbar}\right)^{-\frac{1}{4}+i\frac{z^2}{4\hbar}} \frac{t^{i\frac{z^2}{2\hbar}}}{\sqrt{t}} \exp\left(\frac{it^2}{\hbar}\right)$$

$$\Longrightarrow \phi(t) = \frac{\sqrt{\pi}}{\Gamma\left(\frac{1}{4}+i\frac{z^2}{4\hbar}\right)} \left(\frac{i}{\hbar}\right)^{-\frac{1}{4}+i\frac{z^2}{4\hbar}} \frac{t^{i\frac{z^2}{2\hbar}}}{\sqrt{t}} \exp\left(\frac{it^2}{2\hbar}\right)$$

for $\operatorname{Arg} t = -\frac{\pi}{4}$ or $\frac{3\pi}{4}$. When $t = Te^{-i\frac{3\pi}{4}}$ or $Te^{i\frac{\pi}{4}}$, we must use the series g_1 instead of f_1. We can expect that :

$$\phi(t) = \frac{\sqrt{\pi}}{\Gamma\left(\frac{1}{4}-i\frac{z^2}{4\hbar}\right)} \left(-\frac{i}{\hbar}\right)^{-\frac{1}{4}-i\frac{z^2}{4\hbar}} \frac{t^{-i\frac{z^2}{2\hbar}}}{\sqrt{t}} \exp\left(-\frac{it^2}{2\hbar}\right)$$

for $\operatorname{Arg} t = -\frac{3\pi}{4}$ or $\frac{\pi}{4}$.

5.2 Stokes constants

$$C_S\left(\frac{3\pi}{4}\right) = \left(\frac{1}{\hbar}\right)^{-i\frac{z^2}{2\hbar}} \frac{\Gamma\left(\frac{1}{4}+i\frac{z^2}{4\hbar}\right)}{\Gamma\left(\frac{1}{4}-i\frac{z^2}{4\hbar}\right)} \frac{\left(e^{-i\frac{5\pi}{4}}\right)^{-\frac{1}{2}-i\frac{z^2}{2\hbar}} - \left(e^{-i\frac{\pi}{4}}\right)^{-\frac{1}{2}-i\frac{z^2}{2\hbar}}}{\left(e^{-i\frac{3\pi}{4}}\right)^{-\frac{1}{2}+i\frac{z^2}{2\hbar}}}$$
$$= \left(\frac{1}{\hbar}\right)^{-i\frac{z^2}{2\hbar}} \frac{\Gamma\left(\frac{1}{4}+i\frac{z^2}{4\hbar}\right)}{\Gamma\left(\frac{1}{4}-i\frac{z^2}{4\hbar}\right)} \frac{e^{i\frac{5\pi}{8}}\exp\left(-\frac{5\pi z^2}{8\hbar}\right) - e^{i\frac{\pi}{8}}\exp\left(-\frac{\pi z^2}{8\hbar}\right)}{e^{i\frac{3\pi}{8}}\exp\left(\frac{3\pi z^2}{8\hbar}\right)}$$
$$= \left(\frac{1}{\hbar}\right)^{-i\frac{z^2}{2\hbar}} \frac{\Gamma\left(\frac{1}{4}+i\frac{z^2}{4\hbar}\right)}{\Gamma\left(\frac{1}{4}-i\frac{z^2}{4\hbar}\right)} 2i\sin\left(\frac{\pi}{4}+i\frac{\pi z^2}{4\hbar}\right)\exp\left(-\frac{3\pi z^2}{4\hbar}\right)$$
$$= \left(\frac{1}{\hbar}\right)^{-i\frac{z^2}{2\hbar}} \frac{2i\pi}{\Gamma\left(\frac{1}{4}-i\frac{z^2}{4\hbar}\right)\Gamma\left(\frac{3}{4}-i\frac{z^2}{4\hbar}\right)} \exp\left(-\frac{3\pi z^2}{4\hbar}\right)\,.$$

This last expression can be simplified into :

$$C_S\left(\frac{3\pi}{4}\right) = i\left(\frac{\hbar}{2}\right)^{i\frac{z^2}{2\hbar}} \frac{\sqrt{2\pi}}{\Gamma\left(\frac{1}{2}-i\frac{z^2}{2\hbar}\right)} \exp\left(-\frac{3\pi z^2}{4\hbar}\right)\,,$$

which is exactly the result in [9].

6 Revisiting Landau-Zener, part 2 : when $0 < z \ll \hbar$

By computing the Stokes constants, we are also able to recover the correct behaviour of the scattering matrix $S(z)$ as $z \to 0$. More precisely, we have :

Proposition 1. *Let us consider the vector-valued differential equation :*

$$\frac{\hbar}{i}\frac{d\psi(t)}{dt} = \left[\operatorname{Re}(t+iz)\sigma_3 + \operatorname{Im}(t+iz)\sigma_1\right]\psi(t)$$

being the Landau-Zener problem. When $0 < z \ll \hbar$, the S-matrix is given by :

$$S(z) \underset{0^+}{\sim} \begin{pmatrix} \exp\left(-\frac{\pi z^2}{2\hbar}\right) & -ize^{-i\frac{\pi}{4}}\sqrt{\frac{\pi}{\hbar}}\cosh\frac{\pi z^2}{2\hbar} \\ -ize^{i\frac{\pi}{4}}\sqrt{\frac{\pi}{\hbar}}\cosh\frac{\pi z^2}{2\hbar} & \exp\left(-\frac{\pi z^2}{2\hbar}\right) \end{pmatrix}$$
$$= \exp\left(-\frac{\pi z^2}{2bar}\right)1_2 - iz\sqrt{\frac{\pi}{2bar}}(\sigma_1+\sigma_2)\cosh\frac{\pi z^2}{2bar}\,.$$

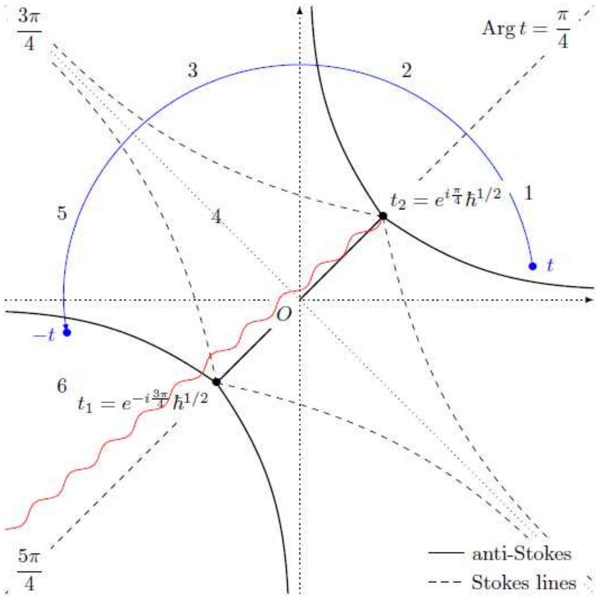

Fig. 2: Stokes structure for 2 simple turning points.

This expression holds continuously as $z \to 0$, *yielding :*

$$\lim_{z\to 0} S(z) = 1_2 \tag{13}$$

$$\textit{and} \quad \frac{dS}{dz}(0) = -i(\sigma_1+\sigma_2)\sqrt{\frac{\pi}{2\hbar}}\,. \tag{14}$$

These transition probabilities can not be valid outside a small neighbourhood of 0, since $\forall z \in \mathbb{R}_+,\ a^2(z)+|b(z)|^2 = 1$, and the factor $z\cosh\dfrac{\pi z^2}{2\hbar}$ shall blow quickly.

6.1 Stokes diagram

The pulsation $Q(t,z) = t^2+z^2-i\hbar$ appears to be a complex number for $t \in \mathbb{R}$. This differential equation displays two turning points that are still first-order zeroes :

$$t \simeq \pm e^{i\frac{\pi}{4}}\hbar^{1/2}\left(1+i\frac{z^2}{2\hbar}\right)$$

since $z \ll \hbar$.

As previously, the asymptotic directions of the Stokes lines are given by $(2k+1)\dfrac{\pi}{4}$. Using the Stokes lines as guides, the remaining elements of the diagram are easily deduced from the properties of the Stokes geometry. Continuation through the upper half-plane gives :

1. start on the positive real axis with the subdominant solution : $(t_2,t)_s$
2. crossing a Stokes line : $(t_2,t)_s$
3. crossing an anti-Stokes line : $(t_2,t)_d$
4. stepping on a Stokes line, using half the Stokes constant : $(t_2,t)_d + \dfrac{C_S}{2}(t,t_2)_s$
   reconnecting while on the line t_2 to t_1 on the left of the cut : $e^{-i\frac{\pi}{2}}[t_2,t_1]_\ell(t_1,t)_d + \dfrac{C_S}{2}(t,t_1)_s[t_1,t_2]_\ell e^{i\frac{\pi}{2}}$
5. stepping off the Stokes line :
   $e^{-i\frac{\pi}{2}}[t_2,t_1]_\ell(t_1,t)_d + (t,t_1)_s\left\{\dfrac{C_S}{2}[t_1,t_2]_\ell e^{i\frac{\pi}{2}} + \dfrac{C_S}{2}e^{-i\frac{\pi}{2}}[t_2,t_1]_\ell\right\}$
6. crossing an anti-Stokes line :
   $e^{-i\frac{\pi}{2}}[t_2,t_1]_\ell(t_1,t)_s + \dfrac{C_S}{2}e^{i\frac{\pi}{2}}\left\{[t_1,t_2]_\ell - [t_2,t_1]_\ell\right\}(t,t_1)_d$
   passing the cut in a counterclockwise sense :
   $e^{-i\frac{\pi}{2}}[t_2,t_1]_\ell(-t,t_1)_s + \dfrac{C_S}{2}e^{i\frac{\pi}{2}}\left\{[t_1,t_2]_\ell - [t_2,t_1]_\ell\right\}(t_1,-t)_d$

where C_S is the Stokes constant associated with the turning point at $t_2 \simeq e^{i\frac{\pi}{4}}\hbar^{1/2}$ and the direction $\operatorname{Arg} t = \dfrac{3\pi}{4}$. The (left) action between the singularities, oriented from $t_1 = e^{i\frac{5\pi}{4}}\hbar^{1/2}\left(1+i\dfrac{z^2}{2\hbar}\right)$ to $t_2 = e^{i\frac{\pi}{4}}\hbar^{1/2}\left(1+i\dfrac{z^2}{2\hbar}\right)$, equals to :

$$W = -\frac{i}{\hbar}\int_{t_1}^{t_2} Q(t)^{1/2}dt = -\frac{i}{\hbar}\int_{t_1}^{t_2}(t^2-i\hbar+z^2)^{1/2}dt\,.$$

Parametrize $t = e^{i\frac{\pi}{4}}\hbar^{1/2}\left(1+i\dfrac{z^2}{2\hbar}\right)\sin\theta$. Then :

$$W \simeq -i\left(1+i\frac{z^2}{2\hbar}\right)^2\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\sqrt{1-\sin^2\theta}\cos\theta\,d\theta$$
$$\simeq -i\left(1+i\frac{z^2}{\hbar}\right)\frac{\pi}{2} = -\frac{i\pi}{2}+\frac{\pi z^2}{2\hbar}$$

which proves to be almost an imaginary number. It is reassuring, since the reconnection path between the turning points is indeed an anti-Stokes line. Thus the factor $[t_1,t_2]_\ell$ is equal to $e^W = -i\exp\left(\dfrac{\pi z^2}{2\hbar}\right)$. One might be surprised at first by the extra i in e^{-W}. Yet since $\hbar$ is no longer negligible, the previous phase factor $t^{\pm i\frac{z^2}{2\hbar}}$ before $\exp\left(\pm\dfrac{it^2}{2\hbar}\right)$ is now replaced by $t^{\pm 1/2}$. An $\pm i$ factor arises naturally, due to the square root presence. Besides, it should be incorporated into the principal parts i.e. in $(t_1,t)_\bullet$ and $(t,t_1)_\bullet$, and not taken into account during the continuation process. That explains the factors $e^{\mp i\frac{\pi}{2}}$ to compensate. Hence :

$$e^{-i\frac{\pi}{2}}e^{-W}(-t,t_1)_s + \frac{C_S}{2}e^{i\frac{\pi}{2}}\left(e^W - e^{-W}\right)(t_1,-t)_d \rightsquigarrow (t_2,t)_s \tag{15}$$

asymptotically speaking.

6.2 Dominant exponential solutions in the $\frac{k\pi}{4}$ directions

In Section 3, we have obtained the coefficients c_{2n} (respectively d_{2n}) in terms of the Gamma function. If we conduct the computations with these exact expressions until the Stokes constant $C_S\left(\frac{3\pi}{4}\right)$, an excellent match is expected. But we will not gain any knowledge of the potential discrepancy. So let us do it the pedestrian way i.e. by keeping only one error term in (7) and (8). We beforehand recall the following result :

Lemma 2. *For any $n \in \mathbb{N}^*$:*

$$\sum_{\ell=0}^{n} \frac{1}{\ell} = \log n + \gamma + \mathcal{O}\left(\frac{1}{n}\right)$$

as well as $$\sum_{\ell=0}^{n-1} \frac{1}{2\ell+1} = \log 2 + \frac{1}{2}(\log n + \gamma) + \mathcal{O}\left(\frac{1}{n}\right)$$

where γ is the Euler-Mascheroni constant.

Recall the expression (7) of the coefficients c_{2k}. Since we assume that $z \ll \hbar$, the general term of f_1 is :

$$c_{2n}t^{2n} = \frac{1}{(2n)!} \prod_{\ell=0}^{n-1} \left[\frac{2i(2\ell+1)}{\hbar} - \frac{z^2}{\hbar^2}\right] t^{2n}$$
$$\simeq \frac{1}{(2n)!} \left[\left(\frac{2i}{\hbar}\right)^n \prod_{\ell=0}^{n-1}(2\ell+1) - \left(\frac{2i}{\hbar}\right)^{n-1} \frac{z^2}{\hbar^2} \prod_{\ell=0}^{n-1}(2\ell+1)\left(1+\frac{1}{3}+\ldots+\frac{1}{2n-1}\right)\right] t^{2n}$$

by neglecting terms of higher order in z^2. Since $\prod_{\ell=0}^{n-1}(2\ell+1) = \frac{(2n)!}{2^n n!}$, we get :

$$c_{2n}t^{2n} \simeq \frac{1}{2^n n!}\left(\frac{2i}{\hbar}\right)^n \left\{1 - \frac{z^2}{2i\hbar}\left[\log 2 + \frac{1}{2}(\log n + \gamma)\right]\right\} t^{2n}$$
$$= \frac{1}{n!}\left(\frac{i}{\hbar}\right)^n \left\{1 + i\frac{z^2}{2\hbar}\left[\log 2 + \frac{1}{2}(\log n + \gamma)\right]\right\} t^{2n} .$$

Approximating a series by an integral :

$$f_1(t) \simeq 1 + \int_1^{+\infty} \frac{1}{x!}\left(\frac{i}{\hbar}\right)^x \left\{1 + i\frac{z^2}{2\hbar}\left[\log 2 + \frac{1}{2}(\log x + \gamma)\right]\right\} t^{2x} dx$$
$$\simeq 1 + \int_1^{+\infty} \frac{1}{\sqrt{2\pi x}}\left(\frac{e}{x}\right)^x \left(\frac{i}{\hbar}\right)^x \left\{1 + i\frac{z^2}{2\hbar}\left[\log 2 + \frac{1}{2}(\log x + \gamma)\right]\right\} t^{2x} dx$$
$$\simeq 1 + \int_1^{+\infty} \frac{1}{\sqrt{2\pi x}}\left(\frac{e}{x}\right)^x \left(\frac{i}{\hbar}\right)^x \left(1 + i\frac{z^2}{4\hbar}\log x\right) t^{2x} dx ,$$

by removing all the small constants $\gamma < \log 2 \ll \frac{1}{2}\log n$ as soon as $n > 4$. With the coefficients d_{2k} in (8), the general term of g_1 becomes :

$$d_{2n}t^{2n} = \frac{(-1)^n}{(2n)!}\frac{z^2}{\hbar^2} \prod_{\ell=1}^{n-1}\left[\frac{2i(2\ell)}{\hbar} + \frac{z^2}{\hbar^2}\right] t^{2n}$$
$$\simeq \frac{(-1)^n}{(2n)!}\frac{z^2}{\hbar^2}\left(\frac{2i}{\hbar}\right)^{n-1} 2^{n-1}(n-1)!\left[1 - i\frac{z^2}{2\hbar}\left(\frac{1}{2}+\frac{1}{4}+\ldots+\frac{1}{2n-2}\right)\right] t^{2n}$$
$$= \frac{(-1)^n}{4in}\frac{n!}{(2n)!}\frac{z^2}{\hbar}\left(\frac{4i}{\hbar}\right)^n \left\{1 - i\frac{z^2}{4\hbar}\left[\log(n-1)+\gamma\right]\right\} t^{2n} .$$

Approximating a series by an integral :

$$g_1(t) \simeq 1 + \frac{z^2}{\hbar}\int_1^{+\infty} \frac{(-1)^x}{4ix}\frac{x!}{(2x)!}\left(\frac{4i}{\hbar}\right)^x \left\{1 - i\frac{z^2}{4\hbar^2}\left[\log(x-1)+\gamma\right]\right\} t^{2x} dx$$
$$\simeq 1 - i\frac{z^2}{4\hbar}\int_1^{+\infty} \frac{(-1)^x}{x}\frac{x!}{(2x)!}\left(\frac{4i}{\hbar}\right)^x \left(1 - i\frac{z^2}{4\hbar}\log x\right) t^{2x} dx$$
$$\simeq 1 - i\frac{z^2}{4\hbar}\int_1^{+\infty} \frac{(-i)^x}{x}\frac{\sqrt{2\pi x}}{\sqrt{4\pi x}}\left(\frac{e}{4x}\right)^x \left(\frac{4}{\hbar}\right)^x \left(1 - i\frac{z^2}{4\hbar}\log x\right) t^{2x} dx$$
$$= 1 - i\frac{z^2}{4\sqrt{2}\hbar}\int_1^{+\infty} \frac{1}{x}\left(-\frac{i}{\hbar}\right)^x \left(\frac{e}{x}\right)^x \left(1 - i\frac{z^2}{4\hbar}\log x\right) t^{2x} dx .$$

In the directions $\operatorname{Arg} t = -\frac{\pi}{4}$ or $\frac{3\pi}{4}$, we shall use the series defining f_1. Set $t = Te^{-i\frac{\pi}{4}}$ or $Te^{i\frac{3\pi}{4}}$:

$$\int_1^{+\infty} \frac{1}{\sqrt{2\pi x}}\left(\frac{e}{x}\right)^x \left(\frac{i}{\hbar}\right)^x \left(1 + i\frac{z^2}{4\hbar}\log x\right) t^{2x} dx$$
$$= \int_1^{+\infty} \frac{1}{\sqrt{2\pi x}}\left(\frac{e}{x}\right)^x \left(1 + i\frac{z^2}{4\hbar}\log x\right)\left(\frac{T^2}{\hbar}\right)^x dx$$
$$\simeq \frac{1}{\sqrt{2\pi x_0}}\left(1 + i\frac{z^2}{4\hbar}\log x_0\right)\int_1^{+\infty} \exp\left(x + x\log\frac{T^2}{\hbar} - x\log x\right) dx$$

where $x_0 = \frac{T^2}{\hbar}$. Therefore, we have :

$$f_1(t) \simeq \left(1 + i\frac{z^2}{4\hbar}\log\frac{T^2}{\hbar}\right)\exp\left(\frac{T^2}{\hbar}\right)$$

since T is large. In other words, the very first summands of both power series of f or g can clearly be neglected. Moreover, we obtain the dominant solutions :

$$\psi_1(t) = \left(1 + i\frac{z^2}{4\hbar}\log\frac{T^2}{\hbar}\right) t^{1/2} \exp\left(\frac{T^2}{2\hbar}\right) .$$

So when $t = Te^{i\frac{3\pi}{4}}$:

$$\psi_1(t) = \left(1 + i\frac{z^2}{4\hbar}\log\frac{e^{-i\frac{3\pi}{2}}t^2}{\hbar}\right) t^{1/2} \exp\left(\frac{it^2}{2\hbar}\right)$$
$$= \left(1 + \frac{3\pi z^2}{8\hbar} + i\frac{z^2}{4\hbar}\log\frac{t^2}{\hbar}\right) t^{1/2} \exp\left(\frac{it^2}{2\hbar}\right) .$$

In the directions $\operatorname{Arg} t = -\frac{3\pi}{4}$ or $\frac{\pi}{4}$, we shall use the series defining g_1 (without the annoying 1) :

$$-i\frac{z^2}{4\sqrt{2}\hbar}\int_1^{+\infty} \frac{(-i)^x}{x}\left(\frac{e}{\hbar x}\right)^x \left(1 - i\frac{z^2}{4\hbar}\log x\right) t^{2x} dx$$
$$\simeq -i\frac{z^2}{4\sqrt{2}\hbar}\frac{1}{x_0}\left(1 - i\frac{z^2}{4\hbar}\log x_0\right)\int_1^{+\infty} \exp\left(x + x\log\frac{T^2}{\hbar} - x\log x\right) dx$$
$$= -i\frac{\sqrt{\pi}z^2}{4\hbar}\sqrt{\frac{\hbar}{T^2}}\left(1 - i\frac{z^2}{4\hbar}\log\frac{T^2}{\hbar}\right)\exp\left(\frac{T^2}{\hbar}\right)$$
$$= -i\frac{z^2}{4}\sqrt{\frac{\pi}{\hbar}}\left(1 - i\frac{z^2}{4\hbar}\log\frac{T^2}{\hbar}\right)\frac{1}{T}\exp\left(\frac{T^2}{\hbar}\right) .$$

And the dominant solutions look like :

$$\psi_1(t) = -i\frac{z^2}{4}\sqrt{\frac{\pi}{\hbar}}\left(1 - i\frac{z^2}{4\hbar}\log\frac{T^2}{\hbar}\right)\frac{t^{-1/2}}{T}\exp\left(\frac{T^2}{2\hbar}\right) .$$

6.3 Stokes constants and transition probabilities

Therefore, we have asymptotically :

- for $\operatorname{Arg} t = \frac{\pi}{4}$:

$$\psi_1(t) = -i\frac{z^2}{4}\sqrt{\frac{\pi}{\hbar}}\left(1 - \frac{\pi z^2}{8\hbar} - i\frac{z^2}{4\hbar}\log\frac{t^2}{\hbar}\right)\frac{e^{i\frac{\pi}{4}}}{t^{3/2}}\exp\left(-\frac{it^2}{2\hbar}\right)$$

- for $\operatorname{Arg} t = \frac{3\pi}{4}$:

$$\psi_1(t) = \left(1 + \frac{3\pi z^2}{8\hbar} + i\frac{z^2}{4\hbar}\log\frac{t^2}{\hbar}\right)t^{1/2}\exp\left(\frac{it^2}{2\hbar}\right)$$

- for $\operatorname{Arg} t = \frac{5\pi}{4}$:

$$\psi_1(t) = -i\frac{z^2}{4}\sqrt{\frac{\pi}{\hbar}}\left(1 - \frac{5\pi z^2}{8\hbar} - i\frac{z^2}{4\hbar}\log\frac{t^2}{\hbar}\right)\frac{e^{i\frac{5\pi}{4}}}{t^{3/2}}\exp\left(-\frac{it^2}{2\hbar}\right).$$

With $z \to 0$ but fixed, it exists T such that $\frac{z^2}{\hbar}\log\frac{T^2}{\hbar} \gg 1$. Henceforth :

- for $\operatorname{Arg} t = \frac{\pi}{4}$:

$$\psi_1(t) = -\frac{z^4}{16\hbar}\sqrt{\frac{\pi}{\hbar}}\log\left(\frac{t^2}{\hbar}\right)\frac{e^{i\frac{\pi}{4}}}{t^{3/2}}\exp\left(-\frac{it^2}{2\hbar}\right)$$

- for $\operatorname{Arg} t = \frac{3\pi}{4}$:

$$\psi_1(t) = i\frac{z^2}{4\hbar}\log\left(\frac{t^2}{\hbar}\right)t^{1/2}\exp\left(\frac{it^2}{2\hbar}\right)$$

- for $\operatorname{Arg} t = \frac{5\pi}{4}$:

$$\psi_1(t) = -\frac{z^4}{16\hbar}\sqrt{\frac{\pi}{\hbar}}\log\left(\frac{t^2}{\hbar}\right)\frac{e^{i\frac{5\pi}{4}}}{t^{3/2}}\exp\left(-\frac{it^2}{2\hbar}\right).$$

Let us compute the Stokes constant at $\frac{3\pi}{4}$:

$$\widetilde{C_S}\left(\frac{3\pi}{4}\right) \simeq \frac{iz^2}{4t}\sqrt{\frac{\pi}{\hbar}}\left(e^{i\frac{5\pi}{4}} - e^{i\frac{\pi}{4}}\right) = -\frac{iz^2}{2t}e^{i\frac{\pi}{4}}\sqrt{\frac{\pi}{\hbar}}.$$

From the Stokes geometry, we know that at $-\infty$, we need a mixed state such that :

$$\begin{aligned}\psi_1(-t) &= e^{-i\frac{\pi}{2}}e^{-W}(-t,t_1)_s + \frac{1}{2}\widetilde{C_S}\left(\frac{3\pi}{4}\right)e^{i\frac{\pi}{2}}\left(e^W - e^{-W}\right)(t_1,-t)_d \\ &= \exp\left(-\frac{\pi z^2}{2\hbar}\right)(-t,t_1)_s - \frac{iz^2}{2t}e^{i\frac{\pi}{4}}\sqrt{\frac{\pi}{\hbar}}\cosh\frac{\pi z^2}{2\hbar}(t_1,-t)_d\end{aligned}$$

since $e^W = -i\exp\left(\frac{\pi z^2}{2\hbar}\right)$. By applying Rule 1 of [10], the S-matrix coefficients are given by :

$$\begin{cases} a(z) = \exp\left(-\frac{\pi z^2}{2\hbar}\right) \\ \widetilde{b}(z) = \frac{2}{z}\frac{iz^2}{2}e^{i\frac{\pi}{4}}\sqrt{\frac{\pi}{\hbar}}\cosh\frac{\pi z^2}{2\hbar} = iz\sqrt{\frac{\pi}{\hbar}}e^{i\frac{\pi}{4}}\cosh\frac{\pi z^2}{2\hbar}\end{cases}.$$

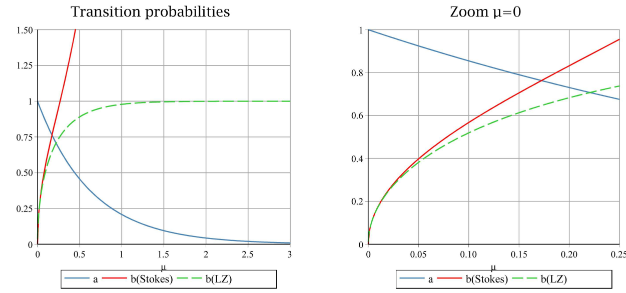

Fig. 3: An approximation in the series' coefficients affects the Stokes constant and gives birth to a discrepancy of $|b(z)|$. For comparison, the theoretical behaviour is plotted in dotted.

Consequently :

$$\frac{d\widetilde{b}}{dz} = i\sqrt{\frac{\pi}{\hbar}}e^{i\frac{\pi}{4}}\left(\cosh\frac{\pi z^2}{2\hbar} + \frac{\pi z^2}{\hbar}\sinh\frac{\pi z^2}{2\hbar}\right)$$

and $$\frac{dS}{dz}(0) = \begin{pmatrix} 0 & -ie^{-i\frac{\pi}{4}} \\ -ie^{i\frac{\pi}{4}} & 0\end{pmatrix}\sqrt{\frac{\pi}{\hbar}} = -i\begin{pmatrix} 0 & 1-i \\ 1+i & 0\end{pmatrix}\sqrt{\frac{\pi}{2\hbar}}.$$

Compare with the result of [8] : $\frac{dS}{dz}(0) = -i(\sigma_1 + \sigma_2)\sqrt{\frac{\pi}{2\hbar}}$!

Define $\mu_1 = \frac{z^2}{\hbar}$. Graphically for $|b(z)|$, our value $\widetilde{C_S}$ gives a pretty nice approximation as long as $z \lesssim 0,15\hbar^{1/2}$.

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