

Chapter 17

A different perspective on the Landau-Zener dynamics

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17.1 Introduction

‘I’ll give you a definite maybe’. This quote by the well-known Polish-born American film producer Samuel Goldwyn, may well be interpreted as a one-line summary of the superposition principle of quantum mechanics. Nowhere clearer do we see quantum interference at work than in the Landau-Zener effect [1–6], with applications ranging from nuclear fission [7] via molecular conical intersections [8] to cold atoms in optical lattices [9–12], matter wave interferometry [13–15] and driven quantum systems [16, 17].

In a recent article [18], we have obtained two ‘one-line derivations’ of the exact Landau-Zener probability amplitude. The first one was based on the Markov approximation [19], and the other on neglecting a second derivative and a deeper understanding of the logarithmic phase singularity. In the present article, we provide a different perspective on the Landau-Zener formula by first expanding on our approach based on the Markov approximation, and then comparing and contrasting it to an amplitude-and-phase approach.

It is a great honor and pleasure for us to dedicate our contribution to this volume to

Professor Victor Dodonov on the occasion of his 75th birthday. Our paths have frequently crossed, and we have learned so much from his asymptotic analysis of the oscillatory photon statistics of a squeezed state, his group theoretical approach towards quantum optics, and his deep insights into the dynamical Casimir effect.

Since at the very heart of Victor's research is asymptotology, we have chosen as the topic for our birthday essay the Landau-Zener effect and hope that it will find his interest. Happy birthday Victor, and many more healthy years in science!

Our article is organised as follows: In Section 17.2 we briefly formulate the problem of Landau-Zener transitions and present the two coupled differential equations of first order for the two probability amplitudes in the interaction picture. Throughout this article we focus on the dynamics of a single probability amplitude.

We dedicate Section 17.3 to a discussion of the approximate but analytic solution of the integro-differential equation for one of the probability amplitudes. This approach provides us with the exact expression for the transition probability amplitude. Moreover, we derive approximate but analytic expressions for the Markov solution, which we compare and contrast to the exact numerical ones. In particular, we establish a relation which connects the integrand of the Markov solution at negative times with positive times. This analysis brings out most clearly the Stueckelberg oscillations.

In Section 17.4 we pursue a different approach and first derive from the integro-differential equation a linear differential equation of second order. We then obtain two coupled differential equations of second order for the absolute value and the phase velocity of the probability amplitude. Although these equations are rather complicated, we can solve them after a linearization. In this way, we make contact with the expressions obtained with the help of the Markov solution.

We conclude by summarizing our results in Section 17.5, and provide a brief outlook.

17.2 Landau-Zener transitions

In the present section we summarize the Landau-Zener problem and introduce dimensional variables. We then present the coupled differential equations for the two probability amplitudes in the Schrödinger as well as in the interaction picture. We conclude by presenting the time dependence of one of them as a trajectory in the complex plane based on a numerical integration of the coupled differential equations.

17.2.1 Formulation of the problem

In its most elementary form the Landau-Zener problem is given by the Schrödinger equation

$$i\hbar \frac{d}{dt} \begin{pmatrix} \tilde{a}(t) \\ \tilde{b}(t) \end{pmatrix} = H(t) \begin{pmatrix} \tilde{a}(t) \\ \tilde{b}(t) \end{pmatrix} \quad (17.1)$$

governed by the time-dependent Hamiltonian

$$\hat{H}(t) = \hbar \begin{pmatrix} -\alpha t & \Omega \\ \Omega & \alpha t \end{pmatrix}. \quad (17.2)$$

Here, α and Ω denote the chirp rate and the coupling constant.

With the dimensionless time $\tau \equiv \Omega \cdot t$, the probability amplitudes $a = a(\tau)$ and $b = b(\tau)$ follow from the set of two coupled differential equations

$$i\dot{\tilde{a}}(\tau) = -\epsilon\tau\tilde{a}(\tau) + \tilde{b}(\tau) \quad (17.3)$$

$$i\dot{\tilde{b}}(\tau) = \tilde{a}(\tau) + \epsilon\tau\tilde{b}(\tau), \quad (17.4)$$

where the dot denotes the differentiation with respect to τ . Here we have introduced the new parameter $\epsilon \equiv \alpha/\Omega^2$ as ratio between the chirp α and the square of the coupling constant Ω .

It is useful to transform from the Schrödinger picture defined by Eq. (17.1) into an interaction picture using the definitions

$$\tilde{a}(\tau) \equiv \exp\left(\frac{i}{2}\epsilon\tau^2\right) a(\tau) \quad (17.5)$$

$$\tilde{b}(\tau) \equiv \exp\left(-\frac{i}{2}\epsilon\tau^2\right) b(\tau), \quad (17.6)$$

which yields the set of coupled differential equations

$$i\dot{a}(\tau) = e^{-i\epsilon\tau^2} b(\tau) \quad (17.7)$$

$$i\dot{b}(\tau) = e^{i\epsilon\tau^2} a(\tau). \quad (17.8)$$

Throughout this article, we consider solutions of these equations for the initial condition

$$a(\tau \rightarrow -\infty) = 1, \quad (17.9)$$

which with the help of the normalization relation

$$|a(\tau)|^2 + |b(\tau)|^2 = 1 \quad (17.10)$$

translates into the initial condition

$$b(\tau \rightarrow -\infty) = 0 \quad (17.11)$$

for the probability amplitude b .

17.2.2 Trajectory of probability amplitude in the complex plane

In Figure 17.1 we depict the time dependence of the probability amplitude a resulting from the numerical integration of the set of equations (17.7) – (17.8) as a trajectory in the complex plane. In this way, we can interpret the motion

$$a(\tau) \equiv A(\tau)e^{i\varphi(\tau)} \quad (17.12)$$

by the time-dependent distance $A \equiv |a(\tau)|$ from the origin and the phase angle $\varphi \equiv \varphi(\tau)$ with respect to the real axis.

Due to the initial condition, Eq. (17.9), the trajectory starts at $\tau = -\infty$ from the value one on the real axis and follows for a long time a circle of radius unity. During this

motion the phase angle φ increases, starting from $\varphi(\tau = -\infty) = 0$. In this domain the phase velocity $\dot{\varphi}$ is negative.

However, in the neighborhood of $\tau = 0$ there is a transition from the initial circle of radius unity to another one whose radius is determined by the final value

$$a(\tau \rightarrow \infty) = \exp\left(-\frac{\pi}{2\epsilon}\right) \quad (17.13)$$

of the probability amplitude given by the Landau-Zener result. Around $\tau = 0$ the phase angle φ assumes a maximum and then decreases again. Obviously, the phase velocity $\dot{\varphi}$ switches from purely negative values to an oscillation between positive and negative values.

Indeed, for positive times, the trajectory performs circular motions, which give rise to the Stueckelberg oscillations. In this regime, the absolute value of a as well as the phase φ oscillate. However, the center of the circles approaches the final radius and the end point of the motion on the real axis. Here, $a(\tau = \infty)$ is real again as indicated by Eq. (17.13).

17.3 Markov approximation

In this section, we decouple the set of equations (17.7) – (17.8), and arrive at an integro-differential equation for the probability amplitude a . When we solve this equation with the help of the Markov approximation [19], we immediately obtain the well-known Landau-Zener formula, Eq. (17.13).

Moreover, we find approximate but analytic results in the limit of large positive and large negative times. These expressions allow us to make the connection to the amplitude and phase approach explored in the next section.

17.3.1 Integro-differential equation

We start the discussion by converting the set of two coupled differential equations of first order for a and b into a integro-differential equation for a . For this purpose, we formally integrate Eq. (17.8) for b subjected to the initial condition, Eq. (17.11), and substitute the result into Eq. (17.7) for a , leading us to the integro-differential equation

$$\dot{a}(\tau) = -e^{-i\epsilon\tau^2} \int_{-\infty}^{\tau} d\tau' e^{i\epsilon\tau'^2} a(\tau') \quad (17.14)$$

with the initial condition given by Eq. (17.9).

On first sight this equation looks rather complicated and no analytic insight offers itself. However, the Markov approximation [19]

$$a(\tau') \approx a(\tau), \quad (17.15)$$

which assumes that the main contribution of the probability amplitude a to the integral in Eq. (17.14) arises from the upper limit, allows us to rederive in essentially one line the Landau-Zener formula, Eq. (17.13). At this point, we do not discuss the validity of this

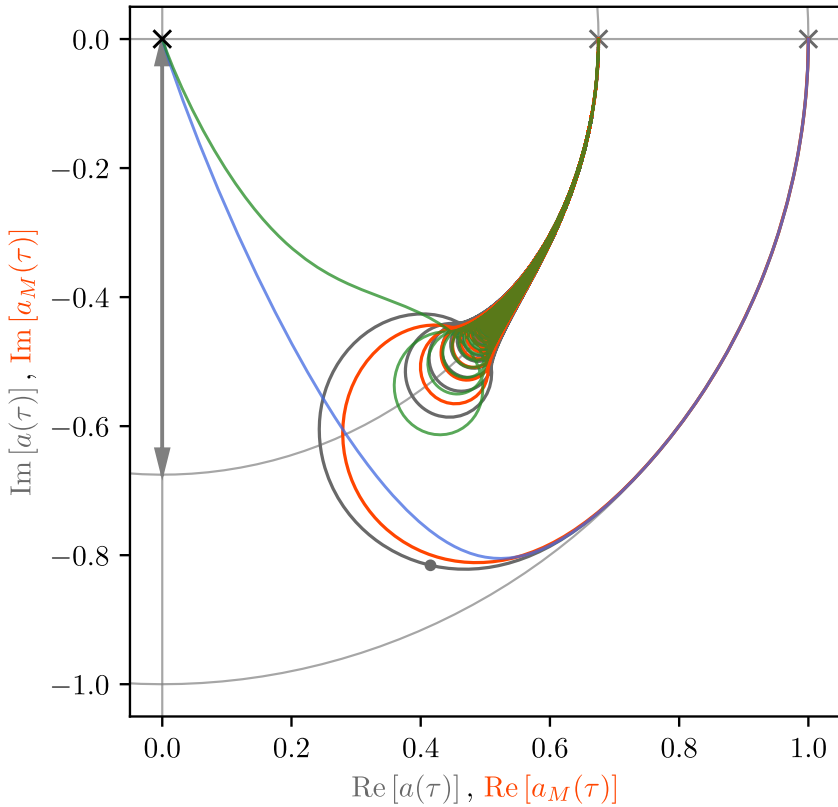


Figure 17.1: Probability amplitudes of a Landau-Zener transition with (red line) and without (dark grey line, numerical solution) the Markov approximation represented in the complex plane for the parameters $\alpha = 0.25$ and $\Omega = 0.25$, that is $\epsilon = 4.0$. The dark grey dot marks $\tau = 0$. Along the trajectory we observe a slight deviation between the numerical and approximated curve especially during the transition from the unit circle to the one with radius (grey arrow) $a(\tau \rightarrow \infty) = \exp(-\pi/(2\epsilon))$. In the limit for $\tau \rightarrow \pm\infty$ both curves agree almost perfectly. The blue and green lines indicate the elementary analytic approximations, Eqs. (17.33) and (17.35), for large negative and positive times. In the neighborhood of the transition, that is $\tau = 0$, the approximation breaks down completely due to the singularity of these approximation of η_M at $\tau = 0$.

approximation, but rather show that in the asymptotic limit of $\tau \rightarrow \infty$ we arrive at the exact result.

Indeed, the Markov approximation allows us to factor a out of the integral and arrive at the equation

$$\dot{a}_M(\tau) = -\eta_M(\tau)a_M(\tau), \tag{17.16}$$

where we have introduced the Markov rate function

$$\eta_M(\tau) \equiv e^{-i\epsilon\tau^2} \int_{-\infty}^{\tau} d\tau' e^{i\epsilon\tau'^2}. \tag{17.17}$$

Here, we have included a subscript M to bring out most clearly that the differential equation (17.16) is an approximation of the exact integro-differential equation (17.14), based on the Markov approximation, Eq. (17.15).

It is straightforward to integrate Eq. (17.16), and we find the Markov solution

$$a_M(\tau) = \exp\left(-\int_{-\infty}^{\tau} d\tau' \eta_M(\tau')\right), \quad (17.18)$$

which satisfies the initial condition, Eq. (17.9).

We conclude by representing the Markov solution, Eq. (17.18), in amplitude and phase, that is

$$a_M(\tau) = A_M(\tau) e^{i\varphi_M(\tau)}, \quad (17.19)$$

where

$$A_M(\tau) \equiv \exp\left(-\int_{-\infty}^{\tau} d\tau' \operatorname{Re}[\eta_M(\tau')]\right) \quad (17.20)$$

and

$$\varphi_M(\tau) = \int_{-\infty}^{\tau} d\tau' \dot{\varphi}_M(\tau') = -\int_{-\infty}^{\tau} d\tau' \operatorname{Im}[\eta_M(\tau')]. \quad (17.21)$$

Here, we have chosen $\varphi(\tau \rightarrow -\infty) = 0$.

Hence, the real part of η_M determines after integration, the amplitude A_M of a_M . In particular, when $\operatorname{Re}[\eta_M]$ is positive, the amplitude decays as a function of time.

The phase φ_M of a_M follows from the integral of the phase velocity $\dot{\varphi}_M$ which is the negative of the imaginary part of η_M . Hence, whenever $\operatorname{Im}[\eta_M]$ is positive, $\dot{\varphi}_M$ is negative, indicating a motion in the clockwise direction.

17.3.2 Exact Landau-Zener formula

The preceding analysis shows that in the Markov approximation, Eq. (17.15), the complete information about the Landau-Zener transition is encoded in the Markov rate function η_M given by Eq. (17.17). For this reason, we will discuss the behavior of η_M in Section 17.3.3 in more detail. However, we first demonstrate that despite the Markov approximation, the asymptotic limit of $a_M(\tau \rightarrow \infty)$ is identical to the exact result, Eq. (17.13).

Indeed, in the asymptotic limit, the Markov solution, Eq. (17.18), reads

$$a_M(\tau \rightarrow \infty) = e^{-I} \quad (17.22)$$

with the integral

$$I \equiv \int_{-\infty}^{\infty} d\tau' e^{-i\epsilon\tau'^2} \int_{-\infty}^{\tau'} d\tau'' e^{i\epsilon\tau''^2}. \quad (17.23)$$

In order to evaluate I , we cast it in the form

$$I = \int_{-\infty}^{\infty} d\tau e^{-i\epsilon\tau^2} \int_{-\infty}^{\infty} d\tau' e^{i\epsilon\tau'^2} - \int_{-\infty}^{\infty} d\tau e^{-i\epsilon\tau^2} \int_{\tau}^{\infty} d\tau' e^{i\epsilon\tau'^2}, \quad (17.24)$$

which with the new integration variables $\bar{\tau} \equiv -\tau$ and $\bar{\tau}' \equiv -\tau'$ in the second integral, and the integral relation

$$\int_{-\infty}^{\infty} d\tau e^{\pm i\epsilon\tau^2} = \sqrt{\frac{(\pm i)\pi}{\epsilon}}, \tag{17.25}$$

reduces to the identity

$$I = \frac{\pi}{\epsilon} - I, \tag{17.26}$$

or

$$I = \frac{\pi}{2\epsilon}, \tag{17.27}$$

and thus yields the exact Landau-Zener formula, Eq. (17.13).

17.3.3 Properties of the Markov rate function

In the preceding subsection, we have obtained an explicit expression, Eq. (17.18), for the Markov solution in terms of the time integral of the Markov rate function η_M defined by Eq. (17.17). In this section, we first derive a linear differential equation of first order, for η_M , and then obtain approximate formulae for large negative and large positive times. Our analysis brings out most clearly that the Stueckelberg oscillations introduce an asymmetry between these time domains.

Differential equation

We start our analysis of η_M by deriving a differential equation for η_M which will become important in the amplitude-and-phase approach pursued in Section 17.4. For this purpose, we differentiate the definition, Eq. (17.17), of η_M and arrive immediately at the linear differential equation

$$\dot{\eta}_M + 2i\epsilon\tau\eta_M - 1 = 0 \tag{17.28}$$

of first order.

The definition (17.17) of η_M also determines the initial condition

$$\eta_M(\tau \rightarrow -\infty) = 0. \tag{17.29}$$

Large negative times

Next, we start from the definition, Eq. (17.17), of η_M and consider large negative times $\tau = -|\tau|$ which yields

$$\eta_M(-|\tau|) = e^{-i\epsilon\tau^2} \int_{|\tau|}^{\infty} d\bar{\tau} e^{i\epsilon\bar{\tau}^2} = e^{-i\epsilon\tau^2} \mathcal{F}(|\tau|). \tag{17.30}$$

Here, we have first introduced the integration variable $\bar{\tau} = -\tau'$ and then the definition

$$\mathcal{F}(\tau) \equiv \int_{\tau}^{\infty} d\bar{\tau} e^{i\epsilon\bar{\tau}^2} \tag{17.31}$$

of the Fresnel integral [20].

From the asymptotic expansion [21]

$$\mathcal{F}(\tau) = \left[-\frac{1}{2i\epsilon\tau} + \frac{1}{4\epsilon^2\tau^3} + \mathcal{O}\left(\frac{1}{\tau^5}\right) \right] e^{i\epsilon\tau^2} \quad (17.32)$$

of \mathcal{F} we find

$$\eta_M(-|\tau|) \approx \frac{1}{4\epsilon^2|\tau|^3} + i\frac{1}{2\epsilon|\tau|}. \quad (17.33)$$

Therefore, for large negative times the real part of η_M is positive and according to Eq. (17.20) the amplitude starts to decrease from unity for decreasing τ . Moreover, the imaginary part of η_M is also positive and leads, due to Eq. (17.21), to a negative phase velocity. Both results are in complete agreement with the numerical integration of the equations of motion shown in Figure 17.1.

Large positive times

For large positive times, we first extend the integration to infinity and then subtract the additional term to arrive at the expression

$$\eta_M(\tau) \equiv e^{-i\epsilon\tau^2} \int_{-\infty}^{\infty} d\tau' e^{i\epsilon\tau'^2} - e^{-i\epsilon\tau^2} \int_{\tau}^{\infty} d\tau' e^{i\epsilon\tau'^2}, \quad (17.34)$$

which reduces with the integral relation, Eq. (17.25), to

$$\eta_M(|\tau|) = -\eta_M(-|\tau|) + \sqrt{\frac{i\pi}{\epsilon}} e^{-i\epsilon\tau^2}. \quad (17.35)$$

In the last step we have compared the second integral to the one in Eq. (17.30).

The relation (17.35) connects the two time domains of large negative and large positive times. Indeed, for large positive times η_M consists of two contributions: (i) A contribution which is identical to negative of η_M at large negative times, and (ii) an oscillatory term with a quadratic phase and a phase shift of $\pi/4$ moving in the complex plane in the clockwise direction as indicated by Figure 17.1.

17.3.4 Landau-Zener probability emerging from Stueckelberg oscillations

The oscillatory term of η_M when integrated over time yields the Stueckelberg oscillations and in the limit of infinite positive time the exact Landau-Zener transition probability, Eq. (17.13). To bring out this fact most clearly, we integrate Eq. (17.35) over positive times only which yields

$$\int_{-\infty}^{\infty} d\tau \eta_M(\tau) = \sqrt{\frac{i\pi}{\epsilon}} \int_0^{\infty} d\tau e^{-i\epsilon\tau^2}. \quad (17.36)$$

Here, we have combined the negative and positive times of η_M into a single integral.

With the help of the integral relation, Eq. (17.25), we arrive at

$$\int_{-\infty}^{\infty} d\tau \eta_M(\tau) = \sqrt{\frac{i\pi}{\epsilon}} \cdot \frac{1}{2} \sqrt{\frac{(-i)\pi}{\epsilon}} = \frac{\pi}{2\epsilon}, \quad (17.37)$$

which is real since the imaginary units compensate each other.

As result, the imaginary part of the Markov rate function η_M must cancel out when integrated over the whole time domain, that is,

$$\int_{-\infty}^{\infty} d\tau \operatorname{Im} [\eta_M] = - \int_{-\infty}^{\infty} d\tau \dot{\varphi}_M = 0. \quad (17.38)$$

Moreover, the corresponding time integral of the oscillations yields a contribution which apart from a factor of $1/2$ is identical to the amplitude of the oscillations given by $\sqrt{\pi/\epsilon}$. The factor $1/2$ is a consequence of the fact that the oscillations only occur for positive times.

We will return to these features in the amplitude-and-phase approach discussed in Section 17.4.

17.3.5 Comparison of Markov solution to the exact probability amplitude

In order to gain insight into the validity of the Markov approximation, we compare and contrast in Figure 17.1 the exact expression for the probability amplitude a , resulting from the numerical integration of the set of equations, Eq. (17.7) and Eq. (17.8), to the Markov solution a_M given by Eq. (17.18).

Due to the initial condition, Eq. (17.9), both trajectories start at $\tau = -\infty$ from the value one on the real axis and are almost indistinguishable following a circle of radius of unity. However, in the neighborhood of $\tau = 0$ where the transition between the two circles takes place, the two trajectories slightly deviate from each other. For positive times both trajectories approach each other again and the final value of $a_M(\tau = \infty)$ agrees with $a(\tau = \infty)$.

17.4 Amplitude and phase approach

In Figure 17.1, we have depicted the time dependence of the probability amplitude a as a trajectory in the complex plane. This representation leads to an intuitive decomposition of a into its amplitude A and phase φ .

In this section, we derive the corresponding coupled equations of motion for A and φ . It is remarkable that one of them can be integrated immediately, and when we substitute its formal solution into the remaining equation of the amplitude-and-phase approach, we arrive at a non-linear differential equation for either φ or A . We conclude this discussion by solving the linearized equation for the phase velocity and make contact with the Markov solution, Eq. (17.18).

17.4.1 Linear second-order differential equation

We start by differentiating the integro-differential equation (17.14) one more time, which leads us immediately to the linear second-order differential equation

$$\ddot{a} + 2i\epsilon\tau\dot{a} + a = 0, \quad (17.39)$$

subjected to the initial conditions, Eq. (17.9) and

$$\dot{a}(\tau \rightarrow -\infty) = 0, \quad (17.40)$$

which follows from Eq. (17.7) in combination with the initial condition, Eq. (17.11), for b .

The solutions of Eq. (17.39) are well known to be the parabolic cylinder functions [21]. Indeed, they are at the very heart of the derivation of the exact Landau-Zener formula, Eq. (17.13). Two linearly independent solutions are needed to satisfy the initial conditions, Eqs. (17.9) and (17.40). In the limit of $\tau \rightarrow \infty$, this combination provides us with the exact result, Eq. (17.13).

In Ref. [18] we have used Eq. (17.39) to obtain another one-line derivation of the exact Landau-Zener expression, Eq. (17.13). For this purpose, we have neglected in Eq. (17.39) the second derivative of a , leading us to the approximate differential equation

$$2i\epsilon\tau\dot{a} = -a. \quad (17.41)$$

Since at $\tau = 0$ the prefactor of \dot{a} vanishes we face a logarithmic phase singularity, in complete analogy to the one of an energy eigenstate of an inverted harmonic oscillator [22] when expressed in terms of quadrature variables [23]. In both cases we arrive in a natural way at the exponential function of Eq. (17.13).

This connection to the inverted harmonic oscillator stands out most clearly when we take the square [24] of the Hamiltonian given by Eq. (17.2). In this way, we arrive [24] at the energy eigenvalue equation of two inverted harmonic oscillators with complex eigenvalues.

Since these aspects of the Landau-Zener problem are not at the center of the present article, we postpone their discussion to a future publication. Nevertheless, we emphasize already now that Eq. (17.41) also provides us with an intriguing connection to Hawking radiation [23].

17.4.2 Equations of motion

In order to solve the linear second-order differential equation (17.39) and establish the connection with the representation (17.12) of a in the complex plane, we make the ansatz

$$a(\tau) \equiv A(\tau)e^{i\varphi(\tau)}, \quad (17.42)$$

where $A(\tau) \equiv |a(\tau)|$.

With the help of the identities

$$\dot{a} = \left(\dot{A} + iA\dot{\varphi} \right) e^{i\varphi} \quad (17.43)$$

and

$$\ddot{a} = \left(\ddot{A} + 2i\dot{A}\dot{\varphi} + iA\ddot{\varphi} - A\dot{\varphi}^2 \right) e^{i\varphi} \tag{17.44}$$

the equation of motion of a , Eq. (17.39), takes the form

$$\ddot{A} + (-\dot{\varphi}^2 - 2\epsilon\tau\dot{\varphi} + 1) A + i \left[A\ddot{\varphi} + 2\dot{A}(\dot{\varphi} + \epsilon\tau) \right] = 0. \tag{17.45}$$

Here, we have already divided by $\exp(i\varphi)$.

When we take the real and imaginary parts of Eq. (17.45) we arrive at the two coupled equations

$$\ddot{A} + (-\dot{\varphi}^2 - 2\epsilon\tau\dot{\varphi} + 1) A = 0 \tag{17.46}$$

and

$$A\ddot{\varphi} + 2\dot{A}(\dot{\varphi} + \epsilon\tau) = 0 \tag{17.47}$$

for the amplitude A and the phase φ of a .

It is interesting that these equations are independent of φ , only derivatives of φ enter. This feature is a consequence of the polar decomposition, Eq. (17.42), of a , that is the fact that φ enters through an exponential function, and the original differential equation (17.39) for a is linear.

The initial condition, Eq. (17.9), translates into

$$A(\tau \rightarrow -\infty) = 1 \tag{17.48}$$

and

$$\varphi(\tau \rightarrow -\infty) = 0. \tag{17.49}$$

Moreover, the initial condition for \dot{a} , Eq. (17.40), implies with Eq. (17.43) the relations

$$\dot{A}(\tau \rightarrow -\infty) = 0 \tag{17.50}$$

and

$$\dot{\varphi}(\tau \rightarrow -\infty) = 0. \tag{17.51}$$

17.4.3 Decoupling the equations of motion

In the preceding section, we have derived the two coupled differential equations, Eqs. (17.46) and (17.47), for the amplitude A and the phase velocity $\dot{\varphi}$. In this section, we decouple them using two different approaches.

For this purpose, we note that Eq. (17.47) is either a homogeneous differential equation of first order for A in terms of $\dot{\varphi}$, $\ddot{\varphi}$ and τ , or an inhomogeneous differential equation of first order for $\dot{\varphi}$ in terms of A , \dot{A} , and τ . In the first case, we obtain with the help of the formal solution $A = A[\dot{\varphi}, \ddot{\varphi}, \tau]$ from Eq. (17.46) a differential equation of second order for $\dot{\varphi}$, whereas in the second case, Eq. (17.46), together with the formal solution $\dot{\varphi} = \dot{\varphi}[A, \dot{A}, \tau]$, yields an integro-differential equation for A .

Equation of motion for phase velocity

In order to decouple the two equations for A and $\dot{\varphi}$, we first note that the ansatz

$$A(\tau) = \exp \left[-\frac{1}{2} \int_{-\infty}^{\tau} d\tau' \frac{\ddot{\varphi}(\tau')}{\dot{\varphi}(\tau') + \epsilon\tau'} \right] \quad (17.52)$$

solves equation (17.47) subjected to the initial condition, Eq. (17.48). However, at this moment it is not obvious that the ansatz, Eq. (17.52), also satisfies the initial condition, Eq. (17.50), for \dot{A} .

In order to address this question, we now differentiate A given in the form

$$A(\tau) = \exp \left[- \int_{-\infty}^{\tau} d\tau' f(\tau') \right], \quad (17.53)$$

where

$$f(\tau) \equiv \frac{1}{2} \frac{\ddot{\varphi}(\tau)}{\dot{\varphi}(\tau) + \epsilon\tau} \quad (17.54)$$

with respect to time which yields

$$\dot{A} = -Af. \quad (17.55)$$

With the initial conditions, Eqs. (17.48) and (17.51), and assuming that for $\tau \rightarrow -\infty$, the phase acceleration $\ddot{\varphi}$ stays finite, we find due to the linear growth of the denominator

$$f(\tau \rightarrow -\infty) = 0, \quad (17.56)$$

and thus the initial condition, Eq. (17.50).

Next, we arrive with the identities

$$\ddot{A} = Af^2 - A\dot{f} \quad (17.57)$$

as well as

$$\dot{f} = \frac{1}{2} \frac{(\dot{\varphi} + \epsilon\tau)\ddot{\varphi} - (\ddot{\varphi} + \epsilon)\dot{\varphi}}{(\dot{\varphi} + \epsilon\tau)^2} \quad (17.58)$$

at the relation

$$\ddot{A} = -\frac{1}{2} \frac{(\dot{\varphi} + \epsilon\tau)\ddot{\varphi} - (3/2\dot{\varphi} + \epsilon)\dot{\varphi}}{(\dot{\varphi} + \epsilon\tau)^2} A. \quad (17.59)$$

When we substitute this formula, Eq. (17.59), into the equation of motion, Eq. (17.46), for A , we arrive at the non-linear differential equation

$$3\ddot{\varphi}^2 - 2(\dot{\varphi} + \epsilon\tau)\ddot{\varphi} + 2\epsilon\dot{\varphi} - 4(\dot{\varphi} + \epsilon\tau)^4 + 4 \left[1 + (\epsilon\tau)^2 \right] (\dot{\varphi} + \epsilon\tau)^2 = 0 \quad (17.60)$$

for the phase φ which is of third order. However, since φ does not appear explicitly, the differential equation is of second order for the phase velocity $\dot{\varphi}$.

Hence, in order to solve the linear differential equation for a , Eq. (17.39), in the representation (17.42) of the amplitude A and the phase φ , we have to proceed in three steps: (i) First we find the solution of the non-linear differential equation of third order for φ . (ii) We then find the expressions $\dot{\varphi}$ and $\ddot{\varphi}$ and substitute them into the formula (17.54) for f . (iii) In the last step, we integrate f over time, which determines by the relation (17.53) the amplitude A .

No pole in the function f

From the definition, Eq. (17.54), of f we note that the denominator of f might vanish, leading to a singularity in f . However, the non-linear differential equation (17.60) for $\dot{\varphi}$ shows that in this case also the numerator given by $\ddot{\varphi}$ vanishes.

Indeed, for times τ_0 when $\dot{\varphi}(\tau_0) + \epsilon\tau_0 = 0$ we find from Eq. (17.60) the relation

$$[3\ddot{\varphi}(\tau_0) + 2\epsilon]\dot{\varphi}(\tau_0) = 0, \quad (17.61)$$

which yields the two conditions

$$3\ddot{\varphi}(\tau_0) + 2\epsilon = 0 \quad (17.62)$$

or

$$\ddot{\varphi}(\tau_0) = 0. \quad (17.63)$$

Equation (17.62) leads to a non-vanishing second derivative of φ , that is,

$$\ddot{\varphi}(\tau_0) = -\frac{2}{3}\epsilon \quad (17.64)$$

and hence to a pole of f . However, as shown in Figure 17.2 not this case, but Eq. (17.63)

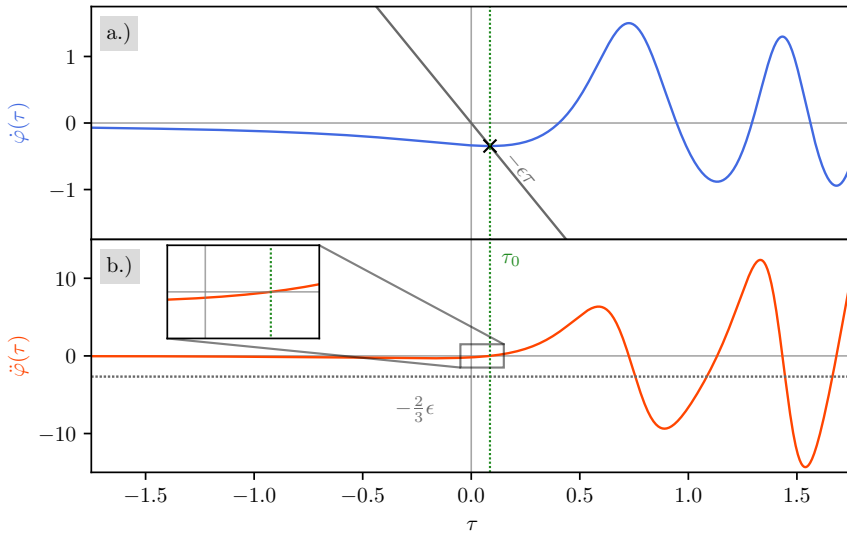


Figure 17.2: No pole in the function f governing the amplitude A of the Landau-Zener transition probability amplitude. a.) The denominator of f given by the sum of the phase velocity $\dot{\varphi}$ and $\epsilon\tau$ has a zero at the time τ_0 indicated by a vertical green dotted line determined geometrically by the crossing of $\dot{\varphi}$ (blue solid line) and a straight line $-\epsilon\tau$ (dark grey solid line). b.) At τ_0 , also $\ddot{\varphi}$ (red solid line) vanishes as shown by the inset. As a result, f does not exhibit a singularity at τ_0 , and in particular, $\ddot{\varphi}$ does not assume the value $-2/3\epsilon$ (dotted grey line) at τ_0 nor in its immediate neighborhood but only at later times.

is realized.

Equation of motion for amplitude

We conclude this discussion of the decoupling of the equations for A and φ by deriving an equation for A by eliminating $\dot{\varphi}$. For this purpose, we cast Eq. (17.47) in the form

$$\ddot{\varphi} = -2\frac{\dot{A}}{A}\dot{\varphi} - 2\frac{\dot{A}}{A}\epsilon\tau \quad (17.65)$$

which with the initial condition, Eq. (17.51), leads us to the formal solution

$$\dot{\varphi}(\tau) = -2\epsilon\frac{1}{A^2(\tau)}\int_{-\infty}^{\tau} d\tau'\tau'A(\tau')\dot{A}(\tau') \quad (17.66)$$

of $\dot{\varphi}$ in terms of A , \dot{A} and τ .

When we substitute this expression into Eq. (17.46) we find a rather complicated integro-differential equation for A which we do not want to present here.

17.4.4 Linearization of equation for phase velocity

In the preceding section, we have decoupled the equations (17.46) and (17.47) for the amplitude A and the phase φ . Unfortunately, the resulting differential equations are very complicated.

However, when we neglect in the differential equation (17.60) the non-linear terms we arrive at a linear differential equation which after another approximation is solved by the negative imaginary part of the Markov rate function η_M . Hence, the Markov solution, Eq. (17.18), is at the very heart of the non-linear differential equation (17.60).

From a non-linear differential equation to a linear one

We start by expanding the terms

$$(\dot{\varphi} + \epsilon\tau)^4 = (\epsilon\tau)^4 + 4(\epsilon\tau)^3\dot{\varphi} + 6(\epsilon\tau)^2\dot{\varphi}^2 + 4\epsilon\tau\dot{\varphi}^3 + \dot{\varphi}^4 \quad (17.67)$$

and

$$(\dot{\varphi} + \epsilon\tau)^2 = (\epsilon\tau)^2 + 2\epsilon\tau\dot{\varphi} + \dot{\varphi}^2 \quad (17.68)$$

in Eq. (17.60) and neglecting all non-linear terms leading us to the approximate expressions

$$(\dot{\varphi} + \epsilon\tau)^4 \approx (\epsilon\tau)^4 + 4(\epsilon\tau)^3\dot{\varphi} \quad (17.69)$$

and

$$(\dot{\varphi} + \epsilon\tau)^2 \approx (\epsilon\tau)^2 + 2\epsilon\tau\dot{\varphi}. \quad (17.70)$$

Hence, Eq. (17.60) reduces to the inhomogeneous linear differential equation

$$\ddot{\varphi}_l - \frac{1}{\tau}\dot{\varphi}_l + \left[(2\epsilon\tau)^2 - 4\right]\dot{\varphi}_l = 2\epsilon\tau \quad (17.71)$$

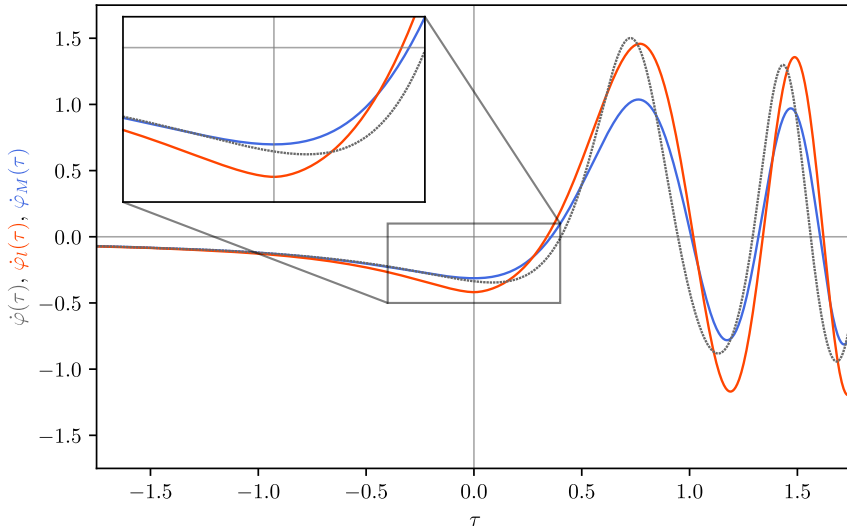


Figure 17.3: Influence of the linearization of the non-linear differential equation (17.60) for the phase velocity $\dot{\varphi}$, and the role of the negative shift of the square of the time variable in the linearized equation (17.71). The solution of the linear differential equation, Eq. (17.71), (red line), displays a behavior similar to the exact numerical curve (dotted grey line). However, there is a disagreement in the amplitudes and phases. The Markov phase velocity, Eq. (17.76), (blue line), which is the exact solution of the linear differential equation, Eq. (17.71), when we neglect the negative shift, that is of Eq. (17.72), does not agree in its maxima nor in its phase with the exact solution either. The deviations of the three curves originate from the different behaviors at $\tau = 0$ amplified in the inset.

of second order for the phase velocity $\dot{\varphi}_l$. Here, we have introduced a subscript l to emphasize the fact that we have linearized Eq. (17.60).

In Figure 17.3, we compare and contrast the numerical solution for the phase velocity $\dot{\varphi}_l$ of Eq. (17.71) represented by the red line with the exact time dependence of $\dot{\varphi}$ given by Eq. (17.60) and shown by the grey dotted line. We note a qualitative but not quantitative agreement.

Connection to the Markov solution

It is interesting that we have already met the exact solution of a differential equation closely related to Eq. (17.71). Indeed, the negative imaginary part of the Markov rate function η_M solves the differential equation

$$\ddot{\varphi}_M - \frac{1}{\tau} \dot{\varphi}_M + (2\epsilon\tau)^2 \dot{\varphi}_M = 2\epsilon\tau, \quad (17.72)$$

that is Eq. (17.71) in absence of the term $-4\dot{\varphi}_l$.

In order to bring this fact out most clearly, we differentiate the differential equation (17.28) of η_M one more time and arrive at the identity

$$\ddot{\eta}_M + 2i\epsilon\eta_M + 2i\epsilon\tau\dot{\eta}_M = 0 \quad (17.73)$$

which with the help of Eq. (17.28) takes the form

$$\ddot{\eta}_M + \frac{1}{\tau}(1 - \dot{\eta}_M) + 2i\epsilon\tau(1 - 2i\epsilon\tau\eta_M) = 0, \quad (17.74)$$

or

$$-\ddot{\eta}_M + \frac{1}{\tau}\dot{\eta}_M - (2\epsilon\tau)^2\eta_M = 2i\epsilon\tau + \frac{1}{\tau}. \quad (17.75)$$

When we take the negative imaginary part of this equation and make the identification $\text{Im}[\eta_M] = -\dot{\varphi}_M$, we arrive at Eq. (17.72).

Hence, the imaginary part of the Markov rate function η_M defined by Eq. (17.17), represents a solution of the differential equation (17.72). Since η_M is given explicitly, the initial conditions are already fixed.

The differential equation for $\dot{\varphi}_M$, Eq. (17.72), is of second order, and thus two initial conditions are necessary. The one for $\dot{\varphi}_M$ translates into one for $-\text{Im}[\eta_M]$, whereas the one for $\ddot{\varphi}_M$ is given by the one for $-\text{Im}[\dot{\eta}_M]$.

As a result,

$$\dot{\varphi}_M = -\text{Im}[\eta_M] \quad (17.76)$$

is a solution of Eq. (17.72) subjected to the initial condition

$$\dot{\varphi}_M(\tau \rightarrow -\infty) = 0 \quad (17.77)$$

following from the initial condition, Eq. (17.29), and

$$\ddot{\varphi}_M(\tau \rightarrow -\infty) = 0 \quad (17.78)$$

given by the asymptotic expansion (17.33) of η_M together with the differential equation (17.28).

In Figure 17.3, we compare and contrast the Markov phase velocity $\dot{\varphi}_M$ given by Eq. (17.76) and of Eq. (17.18) represented by the blue line with the exact time dependence of $\dot{\varphi}$ given by Eq. (17.60) and shown by the grey dotted line. Again we note a qualitative but not quantitative agreement which originates from the time $\tau = 0$ as indicated by the inset.

17.4.5 Decomposition of phase velocity: Anti-symmetric and oscillatory parts

According to Eq. (17.76) the imaginary part of the Markov rate function η_M given by Eq. (17.17) is the exact solution of the differential equation (17.72) subjected to the initial conditions (17.77) and (17.78). However, it is also instructive to find the solutions of the homogeneous and inhomogeneous equation (17.72). Indeed, they are related to the asymptotic expressions, Eqs. (17.33) and (17.35), of η_M .

Solutions of homogeneous and inhomogeneous equation

We first note that the ansatz

$$\dot{\varphi}_h(\tau) \equiv -\mathcal{S} \sin(\beta - \epsilon\tau^2) \quad (17.79)$$

with the two constants \mathcal{S} and β solves the homogeneous equation

$$\ddot{\varphi}_h - \frac{1}{\tau}\dot{\varphi}_h + (2\epsilon\tau)^2\varphi_h = 0. \quad (17.80)$$

Indeed, by differentiation, we find from the identities

$$\ddot{\varphi}_h(\tau) = 2\epsilon\tau\mathcal{S}\cos(\beta - \epsilon\tau^2) \quad (17.81)$$

and

$$\ddot{\varphi}_h(\tau) = 2\epsilon\mathcal{S}\cos(\beta - \epsilon\tau^2) + 4(\epsilon\tau)^2\mathcal{S}\sin(\beta - \epsilon\tau^2) \quad (17.82)$$

that the ansatz φ_h given by Eq. (17.79) satisfies Eq. (17.80). We emphasize that φ_h given by Eq. (17.79) is an *exact* solution of the *homogeneous* equation (17.80).

In contrast, the expression

$$\dot{\varphi}_i(\tau) \equiv \frac{1}{2\epsilon\tau} \quad (17.83)$$

is a particular solution of the inhomogeneous differential equation (17.71) only in the limit of large $|\tau|$.

Indeed, by differentiation, we find from the identities

$$\ddot{\varphi}_i(\tau) = -\frac{1}{2\epsilon\tau^2} \quad (17.84)$$

and

$$\ddot{\varphi}_i(\tau) = \frac{1}{\epsilon\tau^3}, \quad (17.85)$$

and by substitution into the differential equation (17.72) the condition

$$\frac{3}{2\epsilon\tau^3} = 0, \quad (17.86)$$

which is satisfied for large times.

Hence, the complete asymptotic solution is the sum

$$\dot{\varphi}_i(\tau) + \dot{\varphi}_h(\tau) = \frac{1}{2\epsilon\tau} - \mathcal{S}\sin(\beta - \epsilon\tau^2). \quad (17.87)$$

Solutions in different time domains

Since the differential equation (17.72) is of second order, it contains the two constants \mathcal{S} and β of integration. The initial conditions at $\tau \rightarrow -\infty$ determine their values.

Indeed, for large *negative* times, the solution has to satisfy the initial condition (17.51), and hence \mathcal{S} has to vanish, leading us to the expression

$$\dot{\varphi}(-|\tau|) \cong \dot{\varphi}_i(-|\tau|) \cong -\frac{1}{2\epsilon|\tau|}, \quad (17.88)$$

in complete agreement with Eq. (17.33) obtained by the Markov approximation. Here we have explicitly taken into account that τ is negative. We emphasize that in this domain, $\dot{\varphi}$ is solely given by the solution $\dot{\varphi}_i$ of the inhomogeneous equation.

For large *positive* times, the constants of integration \mathcal{S} and β have to be determined by extending the solution from large negative times through $\tau = 0$ to large positive times. In this case \mathcal{S} will not vanish, and we end up with Eq. (17.87).

When we recall from Eq. (17.88) the expression for $\dot{\varphi}$ for large negative times, the solution (17.87) for large positive times takes the form

$$\dot{\varphi}(\tau) = -\dot{\varphi}_i(-|\tau|) - \mathcal{S} \sin(\beta - \epsilon\tau^2), \quad (17.89)$$

which is reminiscent of the imaginary part of Eq. (17.35).

Hence, to this approximation the phase velocity consists of two parts: (i) An anti-symmetric function given by the inhomogeneous solution $\dot{\varphi}_i$, and (ii) an oscillatory function defined by the homogeneous solution $\dot{\varphi}_h$ which only is present for positive times.

Caveats

In the derivation of the linear differential equations (17.71) and (17.72) we have neglected all non-linear terms, such as $\dot{\varphi}^2$ and higher powers, as well as $\ddot{\varphi}^2$ and the product $\dot{\varphi}\ddot{\varphi}$. At this point we have to address the question: Is the resulting solution given by Eq. (17.87) consistent with this approximation?

In order to answer the question we consider the solution (17.79) of the homogeneous equation and evaluate the term

$$\ddot{\varphi}_h^2(\tau) = 4\epsilon^2\tau^2\mathcal{S}^2 \cos^2(\beta - \epsilon\tau^2) \quad (17.90)$$

which we have neglected with the help of Eq. (17.81). Hence, this contribution displays a secular growth.

Moreover, due to the trigonometric relation

$$\cos^2 x = \frac{1}{2} [1 + \cos(2x)], \quad (17.91)$$

the non-linearity creates higher harmonics in the oscillations which are absent in the linearized differential equation, Eq. (17.71), and the Markov rate function, Eq. (17.17). Although, methods [25–27] exist to deal with these two phenomena we do not pursue them in this article.

We conclude the discussion of caveats by bringing out one more peculiarity. The Markov phase velocity $\dot{\varphi}_M$ is an *exact* solution of the *inhomogeneous* equation (17.72), and only in the limit of large times do we find the decomposition into the oscillatory and anti-symmetric part. Hence, from the point of view of the Markov solution, both the oscillatory and the anti-symmetric part originate from the solution of the *inhomogeneous* equation.

In contrast, our elementary analysis solving the inhomogeneous differential equation in the two asymptotic time domains identifies the oscillatory part as the solution of the homogeneous equation, and the anti-symmetric part of the inhomogeneous equation.

This on first sight contradictory picture resolves itself when we include the initial conditions. For large negative times the oscillatory part vanishes but only becomes active for positive times.

17.4.6 Non-linear corrections of the anti-symmetric part of the phase velocity

In the preceding section, we have shown that for large *positive* times the negative phase velocity at large *negative* times enters. This result is based on the inhomogeneous solution $\dot{\varphi}_i$ defined by Eq. (17.83). We devote the present section to show that $\dot{\varphi}_i$ is only the lowest approximation of a non-linear function given by a square root. In this way, we obtain a relation analogous to Eq. (17.89) but including some aspects of the non-linearity of the equations.

Sign change of phase velocity

For this purpose we recall that the numerical integration of the equations of motion leading us to Figure 17.1 shows that for large negative times the amplitude A does not change significantly, and is roughly given by the initial condition (17.48), that is $A(\tau) \approx 1$. For this reason, we can neglect the second derivative of A in Eq. (17.46), that is we set $\ddot{A}(\tau) \approx 0$ which yields

$$(-\dot{\varphi}^2 - 2\epsilon\tau\dot{\varphi} + 1)A \approx 0. \quad (17.92)$$

Since for large negative times the amplitude is approximately the initial condition and therefore non-zero, this condition translates into the relation

$$-\dot{\varphi}^2 - 2\epsilon\tau\dot{\varphi} + 1 = 0. \quad (17.93)$$

When we complete the square, the resulting quadratic equation

$$-(\dot{\varphi} + \epsilon\tau)^2 + (\epsilon\tau)^2 + 1 = 0 \quad (17.94)$$

yields the obvious solutions

$$\dot{\varphi}(\tau) = -\epsilon\tau \pm \sqrt{(\epsilon\tau)^2 + 1}. \quad (17.95)$$

The sign in front of the square root is determined by the initial condition (17.51). Indeed, for large negative times, Eq. (17.95) reduces to

$$\dot{\varphi}(-|\tau|) = \epsilon|\tau| \left[1 \pm \sqrt{1 + \frac{1}{(\epsilon\tau)^2}} \right], \quad (17.96)$$

which with the well-known asymptotic expansion

$$\sqrt{1+x} \approx 1 + \frac{1}{2}x - \frac{1}{8}x^2 \quad (17.97)$$

of a square root gives rise to the expression

$$\dot{\varphi}(-|\tau|) \approx \epsilon|\tau| \left[1 \pm \left(1 + \frac{1}{2(\epsilon\tau)^2} - \frac{1}{8(\epsilon\tau)^4} \right) \right]. \quad (17.98)$$

Hence, only the minus sign leads to the correct initial condition, Eq. (17.51), with the improved approximation

$$\dot{\varphi}(-|\tau|) \approx -\frac{1}{2\epsilon|\tau|} + \frac{1}{8(\epsilon|\tau|)^3}, \quad (17.99)$$

in complete agreement with an naive approach in which we substitute $\dot{\varphi}$ from Eq. (17.88) into $\dot{\varphi}^2$ in Eq. (17.93).

Next we turn to large positive times where Eq. (17.95) takes the form

$$\dot{\varphi}(|\tau|) = \epsilon|\tau| \left[-1 \pm \sqrt{1 + \frac{1}{(\epsilon\tau)^2}} \right]. \quad (17.100)$$

In order to obtain the first term in Eq. (17.89) we need to take the plus sign, that is

$$\dot{\varphi}(|\tau|) \approx \frac{1}{2\epsilon|\tau|} - \frac{1}{8(\epsilon|\tau|)^3}. \quad (17.101)$$

Hence, in this approximation the phase velocity $\dot{\varphi}$ undergoes at $\tau = 0$ a discontinuous jump from negative to positive values. Moreover, this jump seems to be infinite due to a singularity at $\tau = 0$.

The jump in the phase velocity: a red herring

We are now in the position to present an improved approximation for the phase velocity including aspects of the non-linearity of Eq. (17.60). Since for negative times we have to choose the minus sign in front of the square root in Eq. (17.95), we find the expression

$$\dot{\varphi}(-|\tau|) = \mathcal{R}(|\tau|), \quad (17.102)$$

where we have introduced the abbreviation

$$\mathcal{R}(|\tau|) \equiv \epsilon|\tau| - \sqrt{(\epsilon\tau)^2 + 1}. \quad (17.103)$$

Moreover, for positive times we have to select the positive sign in Eq. (17.95), and the function

$$-\epsilon|\tau| + \sqrt{(\epsilon\tau)^2 + 1} = -\mathcal{R}(|\tau|) \quad (17.104)$$

is the improved version of the inhomogeneous solution $\dot{\varphi}_i$.

As a result, Eq. (17.89), including aspects of the non-linearity, takes the form

$$\dot{\varphi}(\tau) = \begin{cases} \mathcal{R}(|\tau|) & \text{for } \tau < 0 \\ -\mathcal{R}(|\tau|) - \mathcal{S} \sin(\beta - \epsilon\tau^2) & \text{for } \tau > 0. \end{cases} \quad (17.105)$$

This analysis suggests that at $\tau = 0$ there is a *finite* jump in $\dot{\varphi}$ from -1 to $1 - \mathcal{S} \sin \beta$ as indicated by Figure 17.4. Obviously this artifact is a consequence of neglecting the second derivative of A . The complete equation, Eq. (17.60), for $\dot{\varphi}$ connects in a continuous and differentiable way the two time domains as shown in Figure 17.4.

Moreover, the square root functions reconfirm the earlier observation that $\dot{\varphi}$ contains an anti-symmetric part, now played by the function \mathcal{R} , and an oscillatory part. The comparison of the exact function including the non-linearity of Eq. (17.60) and the elementary sine function displays a deviation as shown in Figure 17.4.

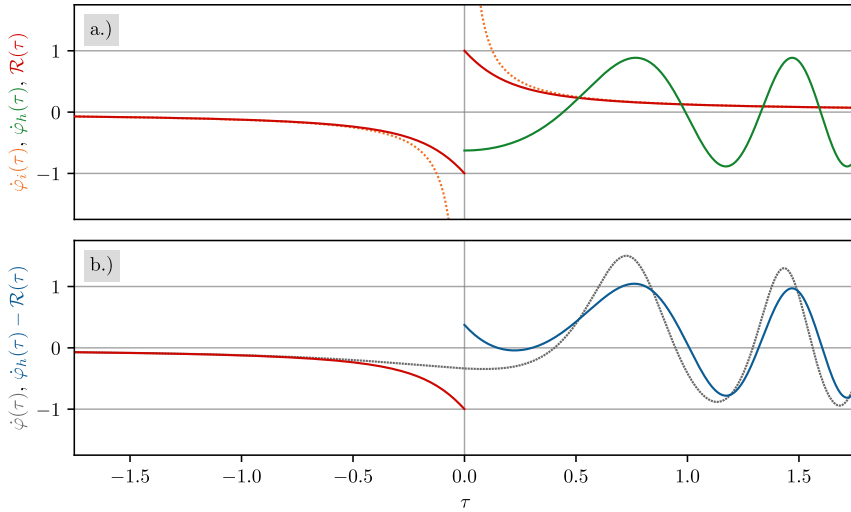


Figure 17.4: Cancellation of phase due to the anti-symmetric part of $\dot{\varphi}$ and the phase shift of $\pi/4$ of the Stueckelberg oscillations a.), and comparison of the exact time dependence of the phase velocity $\dot{\varphi}$ with approximations b.). a.) In the most elementary approximation, the phase velocity $\dot{\varphi}$ is the sum of a square root function \mathcal{R} , given by Eq. (17.103) (red solid line) which is anti-symmetric with respect to the origin, and an sine function with a quadratic phase and a phase shift of $\pi/4$ (green solid line). This oscillatory function appears only for positive times. The area underneath the curve governing the phase of the transition probability amplitude at $\tau = \infty$ vanishes due to the anti-symmetry of \mathcal{R} and the phase shift of the sine function. b.) The exact expression (gray dotted line) connects in a continuous and differentiable way the two approximations for negative times, given by the negative square root, with the one for positive times given by the sum (blue solid line) of the positive square root and the oscillatory term. For large negative and large positive times the inhomogeneous solutions $\dot{\varphi}_i$ given by Eq. (17.83) are the lowest order approximations of \mathcal{R} , as shown in a.) by the orange dotted curve.

17.4.7 Matching the constants of integration

So far we have not specified the constants of integration β and \mathcal{S} which appear in the homogeneous solution $\dot{\varphi}_h$ valid for positive times. Unfortunately, it is impossible to obtain β and \mathcal{S} since we do not have an initial condition in this time domain. However, we now present a heuristic argument based on matching the asymptotic probability amplitude a in amplitude A and phase φ with the Markov solution which is exact.

Determination of phase shift

We start our analysis by considering the phase in the asymptotic limit of an infinite positive time, that is

$$\varphi(\infty) = \int_{-\infty}^{\infty} d\tau \dot{\varphi}(\tau). \tag{17.106}$$

Here, we have taken into account the initial condition (17.49).

Next, we recall from Eq. (17.105) that the phase velocity $\dot{\varphi}$ consists of a sum of an anti-symmetric function and an oscillatory contribution that is only active for positive times. Moreover, the anti-symmetric part is the continuous and differentiable extension of the square root functions \mathcal{R} , given by Eq. (17.103).

Hence, the anti-symmetric part of $\dot{\varphi}$ cancels out in this integral and only the oscillatory part $\dot{\varphi}_h$ for positive times survives, leading us to the expression

$$\varphi(\infty) = \int_0^\infty d\tau \dot{\varphi}_h(\tau) \quad (17.107)$$

which with the help of Eq. (17.79) takes the form

$$\varphi(\infty) = -S\mathcal{I}_s. \quad (17.108)$$

Here, we have introduced the abbreviation

$$\mathcal{I}_s \equiv \int_0^\infty d\tau \sin(\beta - \epsilon\tau^2) = \text{Im} \left[e^{i\beta} \int_0^\infty d\tau e^{-i\epsilon\tau^2} \right]. \quad (17.109)$$

When we recall the integral relation (17.25) we find

$$\mathcal{I}_s = \frac{1}{2} \sqrt{\frac{\pi}{\epsilon}} \text{Im} \left[e^{i(\beta-\pi/4)} \right]. \quad (17.110)$$

Since the numerical integration, in complete agreement with the Markov result, Eq. (17.38), shows $\varphi(\infty) = 0$, we require the choice

$$\beta = \frac{\pi}{4} \quad (17.111)$$

for the constant β of integration.

Determination of amplitude

The condition for β does not specify the amplitude S of the oscillatory term in $\dot{\varphi}_h$. To find S , we first simplify the formula (17.52) for A , consistent with the approximations leading to $\dot{\varphi}_h$.

For this purpose, we recall that the linear differential equation (17.72) emerges from the non-linear differential equation (17.60) when we neglect the non-linear terms. We then perform the integration and match the result to the well-known Landau-Zener formula.

We start from the amplitude

$$A(\infty) = \exp \left[-\frac{1}{2} \int_{-\infty}^\infty d\tau \frac{\ddot{\varphi}(\tau)}{\dot{\varphi}(\tau) + \epsilon\tau} \right] \quad (17.112)$$

in the asymptotic limit of infinite times, and given by Eq. (17.52).

Next, we neglect the non-linearity, that is we drop the term $\dot{\varphi}$ in the denominator which leads us to the expression

$$A(\infty) \equiv \exp \left[-\int_{-\infty}^\infty d\tau' \frac{\ddot{\varphi}(2\tau')}{\epsilon\tau'} \right]. \quad (17.113)$$

The *anti-symmetric* part of the phase velocity leads to a *symmetric* contribution to $\ddot{\varphi}$ which due to the term $\epsilon\tau$ in the denominator makes it into an anti-symmetric function. Hence, this part cancels out in this integral and only the oscillatory part $\dot{\varphi}_h$ for positive parts survives, leading us to the expression

$$A(\infty) \approx \exp \left[- \int_0^\infty d\tau \frac{\ddot{\varphi}_h(\tau)}{2\epsilon\tau} \right]. \quad (17.114)$$

With the help of Eq. (17.81) the asymptotic $A(\infty)$ amplitude takes the explicit form

$$A(\infty) = e^{-S\mathcal{I}_c}, \quad (17.115)$$

where we have introduced the integral

$$\mathcal{I}_c \equiv \int_0^\infty d\tau \cos(\beta - \epsilon\tau^2) = \text{Re} \left[e^{i\beta} \int_0^\infty d\tau e^{-i\epsilon\tau^2} \right]. \quad (17.116)$$

We again recall the integral relation, Eq. (17.25), and find

$$\mathcal{I}_c = \frac{1}{2} \sqrt{\frac{\pi}{\epsilon}} \text{Re} \left[e^{i(\beta - \pi/4)} \right], \quad (17.117)$$

which with the expression (17.111) for the phase shift β reduces to

$$\mathcal{I}_c = \frac{1}{2} \sqrt{\frac{\pi}{\epsilon}}. \quad (17.118)$$

When we match the product $S\mathcal{I}_c$ with the exact asymptotic result I given by Eq. (17.27), we obtain the condition

$$\mathcal{S} \cdot \frac{1}{2} \sqrt{\frac{\pi}{\epsilon}} = \frac{\pi}{2\epsilon} \quad (17.119)$$

which leads us to the expression

$$\mathcal{S} = \sqrt{\frac{\pi}{\epsilon}} \quad (17.120)$$

for the amplitude \mathcal{S} of the oscillatory term.

Summary

This approach brings out most clearly that the final Landau-Zener probability amplitude is the result of three features: (i) The oscillatory term of the phase velocity has the amplitude \mathcal{S} given by Eq. (17.120), varies quadratically in time, and has a phase shift of $\pi/4$. (ii) The probability amplitude is an integral over positive times only, and (iii) the integration yields another factor $\mathcal{S}/2$.

In the language of John A. Wheeler this interpretation takes the form

$$\left(\begin{array}{c} \text{Landau-} \\ \text{Zener} \\ \text{probability} \\ \text{amplitude} \end{array} \right) = \exp \left[- \left(\begin{array}{c} \text{amplitude} \\ \text{of} \\ \text{oscillations} \\ \text{in phase velocity} \end{array} \right) \times \left(\begin{array}{c} \text{integral} \\ \text{over} \\ \text{quadratic} \\ \text{phase} \end{array} \right) \right], \quad (17.121)$$

that is

$$a(\infty) = \exp \left[-\mathcal{S} \cdot \frac{1}{2} \mathcal{S} \right], \quad (17.122)$$

where the factor $1/2$ reflects the fact that the integration extends only over positive times.

17.5 Conclusion and outlook

In the present article, we have revisited the well-known problem of Landau-Zener transitions. Here, we have first recalled the essential ingredients of our recent approach [18] based on the Markov approximation. The corresponding integro-differential equation for the probability amplitude a reduces to the elementary differential equation of an exponential function when we factor a out of the integral. The essence of the Markov approximation is the dependence of the probability amplitude at time τ solely on τ , and not on the values at previous times. This, at first sight, dramatic approximation provides us not only with the exact asymptotic Landau-Zener value, but also connects the behavior of the probability amplitude at large negative times with the one at large positive times with the help of Fresnel integrals. When we evaluate these integrals for large positive and negative times, we obtain approximate but analytic expressions for the probability amplitude.

We have complemented the Markov approach by one based on a decomposition of the probability amplitude into its amplitude and phase. The resulting equations of motion are coupled but lead, when decoupled, to rather complicated equations for only the amplitude and only the phase. However, when we neglect the non-linear terms, or consider the asymptotic limit of large negative and large positive times, we can solve these equations approximately and confirm the analytic expressions obtained by the Markov technique.

However, there is a subtlety. In contrast to the Markov solution, we now do not have an analytic expression that connects the two asymptotic time domains. We have to solve the differential equations in the two different regimes separately. This complication is not a problem for large negative times since we have the initial condition to fix the solution. However, it is a problem for large positive times. Here, the approach cannot determine the phase and the amplitude of the Stueckelberg oscillations. These constants can only be obtained by a comparison to the Markov approximation.

Obviously, many questions remain. It suffices to name three.

The amplitude-and-phase approach yields results identical to the Markov solution when we neglect the non-linearity. Hence, there must be a strong connection between linearization and Markov approximation, but what is this connection and why does the Markov solution provide us still with the exact result neglecting the non-linearity.

So far, we have only focused on the probability amplitude a , and we may ask the following question: Do our techniques lead to meaningful results when applied to the probability amplitude b ?

Finally, a major complication of the Landau-Zener problem is the time dependence of the Hamiltonian (17.2), requiring time-ordering of the corresponding Dyson series. However, in an unpublished article [28] A. G. Rojo has demonstrated by an elegant evaluation of the high-dimensional coupled integrals that the Dyson sum is just the exponential of the familiar Landau-Zener result. Unfortunately, Rojo did not point out the deeper

symmetry, which made this calculation possible. Is it contained in the rapidly varying quadratic phase factors or in an attractor of the set of differential equations?

Although we have gained many insights into and numerous answers to some aspects of these questions, it still represents work in progress. Therefore, we have to postpone the publication of these answers to the 150th birthday of Victor.

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