

## Superadiabatic tracking of quantum evolution

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1991 J. Phys. A: Math. Gen. 24 3255

(<http://iopscience.iop.org/0305-4470/24/14/014>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 01/06/2010 at 11:02

Please note that [terms and conditions apply](#).

## Superadiabatic tracking of quantum evolution

R Lim and M V Berry

H H Wills Physics Laboratory, Tyndall Avenue, Bristol BS8 1TL, UK

Received 20 March 1991

**Abstract.** The adiabatic quantum evolution of a two-state system without energy-level crossings is an example of the Stokes phenomenon. In the latter, a small (subdominant) exponential in an asymptotic expansion appears when a Stokes line is crossed; truncating the dominant asymptotic series at its least term causes the multiplier of the subdominant term to rise in a smooth, compact and universal manner across the Stokes line. In quantum evolution this corresponds to a smooth transition, universal in form, between 'superadiabatic' basis states (high-order WKB approximate solutions of the time-dependent Schrödinger equation). We give a numerical demonstration of this previously predicted universality by constructing, for two Hamiltonians, the superadiabatic quantum bases asymptotic to the actual evolving state. Universality when a Stokes line is crossed is seen in the changing probability that the system makes a transition away from the superadiabatic state, and occurs at that order of superadiabatic approximation corresponding to truncating the asymptotic series at its least term.

### 1. Introduction

Our purpose is to give numerical illustrations of a recent theory (Berry 1990b, hereinafter called I) for the time development (history) of quantum transitions induced by a slowly-changing Hamiltonian  $\hat{H}(\tau)$ . That theory was stimulated by recent progress in understanding the Stokes phenomenon of asymptotics (Berry 1989, 1990a). In I, the central prediction was that if the evolving quantum state is tracked in a particular 'optimal superadiabatic' basis, the rise in the amplitude for transition to an initially unoccupied state, from zero to the final exponentially small value, has a universal form given by an error function.

The optimal superadiabatic basis is one of a sequence of superadiabatic bases, whose lowest member is the ordinary adiabatic basis, consisting of the instantaneous eigenstates of  $\hat{H}$ . Higher members of the sequence are successive truncations of the (divergent) asymptotic series solution of the time-dependent Schrödinger equation in powers of the adiabatic parameter  $\epsilon$ . As is well known (e.g. Landau and Lifshitz 1977), none of these truncations describes transitions from the initial state, because such transitions are exponentially weak, that is 'beyond all orders' in  $\epsilon$ . Any of them can, however, be employed as a basis to describe the exact evolution. The optimal basis corresponds to truncation of the asymptotic series at its least term (whose order is proportional to  $\epsilon^{-1}$ ). In section 2 we summarize the construction of this family of bases; details can be found in I.

Universality emerges when high-order bases are employed, and is a consequence of the existence of degeneracies in the complex-time plane. As summarized in section 3, at the optimal order universality takes the form of the transition amplitude reaching its exponentially small final value by adhering closely to the error function of a natural

variable; again, details can be found in I. At the optimal order there are oscillatory deviations from the error function which, however, vanish in the adiabatic limit; these too are universal in form. Beyond the optimal order, the transition histories rapidly acquire wild oscillations, and the error function no longer applies.

This 'transitory renormalization' as we move along the sequence of superadiabatic bases, onto the universal error-function history, is an unfamiliar and interesting phenomenon, worth illustrating. For this we employ two model Hamiltonians. As described in section 4, these are the Landau-Zener model (Zener 1932), and a variant of this. For each, the superadiabatic bases are constructed, and the transition histories calculated exactly and compared with the predictions of the asymptotic theory of I.

## 2. Superadiabatic bases

We wish to solve the Schrödinger equation

$$i\varepsilon \frac{d}{d\tau} |\psi(\tau)\rangle = \hat{H}(\tau) |\psi(\tau)\rangle \quad |\psi(\tau)\rangle = \begin{pmatrix} \psi_{\text{up}}(\tau) \\ \psi_{\text{down}}(\tau) \end{pmatrix} \quad (1)$$

involving the 'slow time'  $\tau$  and the (small) adiabatic parameter  $\varepsilon$  (which incorporates Planck's constant  $\hbar$ ). For  $\hat{H}$  we can take a real symmetric  $2 \times 2$  matrix:

$$\hat{H}(\tau) = \begin{pmatrix} Z(\tau) & X(\tau) \\ X(\tau) & -Z(\tau) \end{pmatrix} = H(\tau) \begin{pmatrix} \cos\{\theta(\tau)\} & \sin\{\theta(\tau)\} \\ \sin\{\theta(\tau)\} & -\cos\{\theta(\tau)\} \end{pmatrix}. \quad (2)$$

It is helpful to regard the time development of  $\hat{H}$  as a path in the plane with Cartesian coordinates  $X, Z$  and polar coordinates  $H, \theta$ . The path is analytic, and may not pass through the origin—that is,  $\hat{H}$  is not degenerate for any real time. The energy levels are  $\pm H(\tau)$  and the adiabatic (instantaneous) eigenstates are, in an obvious notation,

$$|+(\tau)\rangle = \begin{pmatrix} \cos \frac{1}{2}\theta(\tau) \\ \sin \frac{1}{2}\theta(\tau) \end{pmatrix} \quad |-(\tau)\rangle = \begin{pmatrix} \sin \frac{1}{2}\theta(\tau) \\ -\cos \frac{1}{2}\theta(\tau) \end{pmatrix}. \quad (3)$$

Initially, the system is in the  $+$  state, that is  $|+(\tau \rightarrow -\infty)\rangle$ . We seek the history of the amplitude for transitions away from this state—or rather, from states that cling superadiabatically to this state as it changes with  $\hat{H}(\tau)$ . Thus we write

$$|\psi(\tau)\rangle = c_{n+}(\tau) |\psi_{n+}(\tau)\rangle + c_{n-}(\tau) |\psi_{n-}(\tau)\rangle \quad (4)$$

where  $|\psi_{n\pm}(\tau)\rangle$  are the superadiabatic basis states at the  $n$ th order, whose construction will soon be described. The zero-order states are proportional to the ordinary adiabatic states  $|\pm(\tau)\rangle$  defined in (3). The desired transition amplitude is thus

$$c_{n-}(\tau) = \langle \psi_{n-}(\tau) | \psi(\tau) \rangle \quad (5)$$

with the initial conditions in (3) being  $c_{n-}(-\infty) = 0$ ,  $c_{n+}(-\infty) = 1$ . The transition probability is  $|c_{n-}(\tau)|^2$ .

Clearly the determination of  $c_{n-}$  requires the superadiabatic states with lower energy  $-H(\tau)$ , namely  $|\psi_{n-}\rangle$ ; these are approximations to the state orthonormal to the evolving state. The  $n$ th such superadiabatic state is the formal series solution of the Schrödinger equation in powers of  $\varepsilon$ , truncated at the term in  $\varepsilon^n$ , namely

$$|\psi_{n-}(\tau)\rangle = \exp\left\{\frac{i}{\varepsilon} \int_0^\tau H(\tau') d\tau'\right\} \sum_{m=0}^n \varepsilon^m [\alpha_m(\tau) |+(\tau)\rangle + \beta_m(\tau) |-(\tau)\rangle]. \quad (6)$$

For a given Hamiltonian path, specified by the functions  $H(\tau)$  and  $\theta(\tau)$ , the coefficient functions  $\alpha_m(\tau)$  and  $\beta_m(\tau)$  are determined by recursion, as follows:

$$\alpha_0(\tau) = 0 \quad \beta_0(\tau) = 1 \quad \alpha_1(\tau) = \frac{i}{4H(\tau)} \frac{d\theta(\tau)}{d\tau}$$

$$\alpha_{m+1}(\tau) = \frac{i}{2H(\tau)} \left[ \frac{d\alpha_m(\tau)}{d\tau} + \frac{1}{4} \frac{d\theta(\tau)}{d\tau} \int_{-\infty}^{\tau} d\tau' \frac{d\theta(\tau')}{d\tau'} \alpha_m(\tau') \right] \quad (m \geq 1) \quad (7)$$

$$\beta_m(\tau) = \frac{1}{2} \int_{-\infty}^{\tau} d\tau' \frac{d\theta(\tau')}{d\tau'} \alpha_m(\tau') \quad (m \geq 1).$$

These conditions ensure that the superadiabatic states correspond to the lower, rather than the upper, energy eigenstate, and also that the states are orthogonal to order  $\epsilon^{n+1}$ . (Note that similar formulae in I refer to the upper superadiabatic states  $|\psi_{n+}\rangle$ .)

### 3. Universal transition histories

Given any Hamiltonian path and an exact solution of the corresponding Schrödinger equation (1), the prescription for calculating the transition amplitude  $c_-(\tau)$  is projection, according to (5), onto the superadiabatic state defined by equations (6) and (7). In the analytic theory (I) of the universal transition amplitude, two further ingredients enter.

The first is the large-order behaviour of the coefficient functions  $\alpha_m(\tau)$ . Because of the form of the recursion (7), this is determined by the singularities of the lowest-order function  $\alpha_1(\tau)$  which are closest to the real  $\tau$  axis: the successive differentiations magnify the singularities, whose domain of influence swells so as eventually (that is, for large  $m$ ) to reach the real  $\tau$  axis. The singularities are the *complex degeneracies*, that is complex zeros of  $H(\tau)$ ; they occur in conjugate pairs. From the form of  $\alpha_1(\tau)$  in (7) an obvious natural variable is

$$w(\tau) \equiv 2 \int_0^{\tau} d\tau' H(\tau'). \quad (8)$$

This variable has a further significance: it is the difference between the phase of the exponent in (6) and the corresponding phase in the upper superadiabatic states, that is the disparity between the phases in the two contributions to the superposition (4). The fact that the superposition involves two competing exponentials makes it unsurprising that the Stokes phenomenon will appear.

Let the nearest singularity in the lower half-plane be  $w_c$ . Then close to  $w_c$  the appropriate limiting form can be calculated to be

$$\frac{1}{2H(\tau)} \frac{d\theta(\tau)}{d\tau} \approx \frac{i}{3(w - w_c)} \quad \text{i.e. } \alpha_1(\tau) \approx -\frac{1}{6(w - w_c)}. \quad (9)$$

By recursion this generates large-order coefficients which, when combined with their counterparts for the conjugate singularity  $w_c^*$ , lead to

$$\alpha_m(\tau) \xrightarrow{m \rightarrow \infty} \frac{(-i)^{m+1} (m-1)!}{2\pi} \left[ \frac{1}{(w - w_c)^m} - \frac{1}{(w - w_c^*)^m} \right]. \quad (10)$$

Each term shows the 'factorial divided by power' divergence typical of an asymptotic expansion (Dingle 1973).

The second ingredient is the use of perturbation theory to calculate the transition amplitude. As explained in I (see also Berry 1990a), this would not be justified for low-order bases but is valid for large  $n$ . Perturbation theory, applied to the Schrödinger equation in the  $n$ th superadiabatic basis, gives

$$c_{n-}(\tau) \approx -i(-\varepsilon)^n \int_{-\infty}^{w(\tau)} dw \alpha_{n+1}(\tau(w)) \exp(-iw/\varepsilon). \quad (11)$$

Combining these two ingredients, we obtain

$$c_{n-}(\tau) \approx \frac{i^{n+1} \varepsilon^n n!}{2\pi} \int_{-\infty}^{w(\tau)} dw \exp(-iw/\varepsilon) \left[ \frac{1}{(w-w_c)^{n+1}} - \frac{1}{(w-w_c^*)^{n+1}} \right]. \quad (12)$$

It is convenient, and involves no loss of generality, to make  $w_c$  purely imaginary ( $\equiv -i|w_c|$ ). This simply amounts to an appropriate shift in the origin  $\tau=0$ , to make this correspond to the instant when a *Stokes line* issuing from  $w_c$  crosses the real  $\tau$  axis. (Stokes lines are defined by  $\text{Re}(w-w_c)=0$ .) Then the expansion of the fractions in (12) to second order in  $|w/w_c|$  leads to

$$c_{n-}(\tau) \approx \frac{n!}{2\pi|w_c|} \left( \frac{\varepsilon}{|w_c|} \right)^n \int_{-\infty}^{w(\tau)} dw \exp \left\{ -\frac{(n+1)w^2}{2|w_c|^2} \right\} \\ \times \left[ \exp \left\{ \frac{-iw}{\varepsilon} \left( 1 - \frac{\varepsilon(n+1)}{|w_c|} \right) \right\} + (-1)^n \exp \left\{ \frac{-iw}{\varepsilon} \left( 1 + \frac{\varepsilon(n+1)}{|w_c|} \right) \right\} \right]. \quad (13)$$

The first exponential in the square brackets oscillates more slowly than the second, and as a first approximation we may disregard the latter. The prefactor is smallest for  $n \sim |w_c|/\varepsilon$ , and this same choice almost removes the oscillations in the integrand, leaving a Gaussian integrand. Thus, after using Stirling's formula, we obtain the error function

$$c_{n-}(\tau) \approx \frac{1}{2} [1 + \text{erf}\{\sigma(\tau)\}] \exp(-|w_c|/\varepsilon) \quad \text{for } n \approx |w_c|/\varepsilon$$

where

$$\sigma(\tau) \equiv w(\tau)/\sqrt{2\varepsilon|w_c|}. \quad (14)$$

This has the now-familiar form for the switching on of a subdominant exponential across a Stokes line (Berry 1989, 1990a). The argument  $\sigma$  of the error function is the Stokes variable (Berry 1989), namely the imaginary part of the 'singulant' (difference between the two exponents) divided by the square root of twice the singulant. The formula (14) also gives the correct exponential small final transition probability.

#### 4. Two model Hamiltonians

We now obtain the transition histories for two models for which it is possible to solve (4) and (5) and hence obtain the functions  $\alpha_m$  and  $\beta_m$ . The first is the well known *Landau-Zener Hamiltonian* (Zener 1932)

$$Z(\tau) = \tau \quad X(\tau) = 1. \quad (15)$$

The polar angle  $\theta(\tau)$  decreases from  $\pi$  to 0,

$$\frac{1}{H(\tau)} \frac{d\theta(\tau)}{d\tau} = -\sin^3 \theta(\tau) \tag{16}$$

and

$$w(\tau) = \tau\sqrt{1+\tau^2} + \ln(\sqrt{1+\tau^2} + \tau) = \cot \theta \operatorname{cosec} \theta + \ln(\cot \theta + \operatorname{cosec} \theta). \tag{17}$$

The degeneracies occur at  $\tau = \pm i$ , giving  $w_c = -i\pi/2$ .

Our second model, which we call the *tanh Hamiltonian*, is similar to Landau-Zener but its energy spacing remains finite as  $\tau \rightarrow \pm\infty$ :

$$Z(\tau) = \tanh \tau \quad X(\tau) = 1. \tag{18}$$

The polar angle  $\theta(\tau)$  now decreases from  $3\pi/4$  to  $\pi/4$ ,

$$\frac{1}{H(\tau)} \frac{d\theta(\tau)}{d\tau} = \sin \theta(\tau) \cos 2\theta(\tau) \tag{19}$$

and

$$\begin{aligned} w(\tau) &= 2\sqrt{2} \sinh^{-1}(\sqrt{2} \sinh \tau) - 2 \sinh^{-1}(\tanh \tau) \\ &= 2\sqrt{2} \log(1 + \sqrt{2} \cos \theta) - \sqrt{2} \log(-\cos 2\theta) + 2 \log(\cot \theta + \operatorname{cosec} \theta). \end{aligned} \tag{20}$$

Now there is a string of degeneracies, at  $\tau = \pm i(2n + 1)\pi/4$ ; the nearest to the real axis has  $w_c = -i\pi(\sqrt{2} - 1)$ .

For both Hamiltonians, we constructed the superadiabatic bases by calculating the functions  $\alpha_m$  and  $\beta_m$  from (7), using for convenience the variable  $\theta$  rather than  $\tau$ . This is a tedious affair, with the coefficients in the results soon swelling to unwieldy proportions, as manual calculation of the first few will confirm. Fortunately the advent of powerful symbolic computational packages obviates the need for such effort. We used the package Mathematica to generate these functions (and also for the rest of the numerical work in this paper).

To find the transition amplitudes  $c_{n-}(\tau)$  from the projection (5), it is also necessary to solve the Schrödinger equation. For the Landau-Zener model the exact solution of (1) starting out in the spin-down state (which as  $\tau \rightarrow -\infty$  is the higher-energy state) can be expressed in terms of parabolic cylinder functions (Gradshteyn and Ryzhik 1980):

$$|\psi(\tau)\rangle = \exp\left\{-\frac{\pi}{8\varepsilon}\right\} \begin{pmatrix} -i\pi\nu^{1/2} D_{\nu-1}\{\zeta(\tau)\} \\ D_{\nu}\{\zeta(\tau)\} \end{pmatrix} \tag{21}$$

where  $\nu \equiv i/2\varepsilon$  and  $\zeta(\tau) \equiv \tau\sqrt{2/\varepsilon} \exp(3\pi i/4)$ . For the tanh model, we solved the matrix equation (1) numerically, by Runge-Kutta integration.

Because we seek to display the predicted universality, we choose the values of  $|w_c|/\varepsilon$  to be the same for both models, namely 5.205. Thus the final transition amplitude is

$$|c_{n-}(+\infty)| = \exp\left(-\frac{|w_c|}{\varepsilon}\right) = 0.0055 \dots \tag{22}$$

The expected optimal order of superadiabaticity, giving the error-function amplitude (14), is  $n = 5$ . The corresponding adiabatic parameters are  $\varepsilon = 0.3018$  for the Landau-Zener model and  $\varepsilon = 0.25$  for the tanh model.

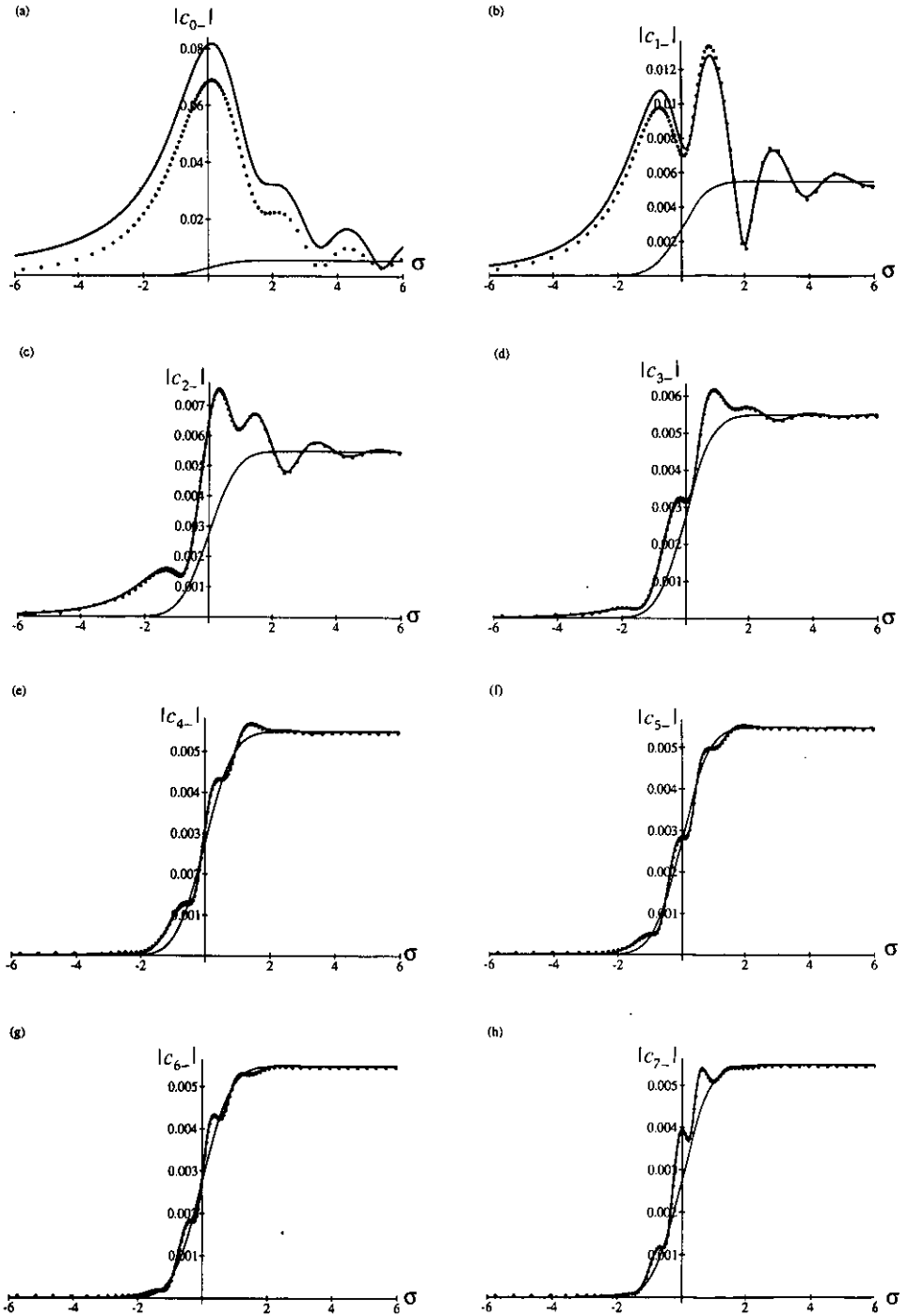


Figure 1. (a)-(k). Sequence of histories of transition amplitudes  $|c_{n-}(\tau(\sigma))|$  in (a) the ordinary adiabatic basis  $n=0$  and (b)-(k) the superadiabatic bases  $n=1-10$ , for the Landau-Zener Hamiltonian with  $\epsilon=0.3018$  (thick line) and the tanh Hamiltonian with  $\epsilon=0.25$  (dots). The thin line is the optimal superadiabatic error function (14), which as expected best fits the data for  $n=5$  (figure 1(f)).

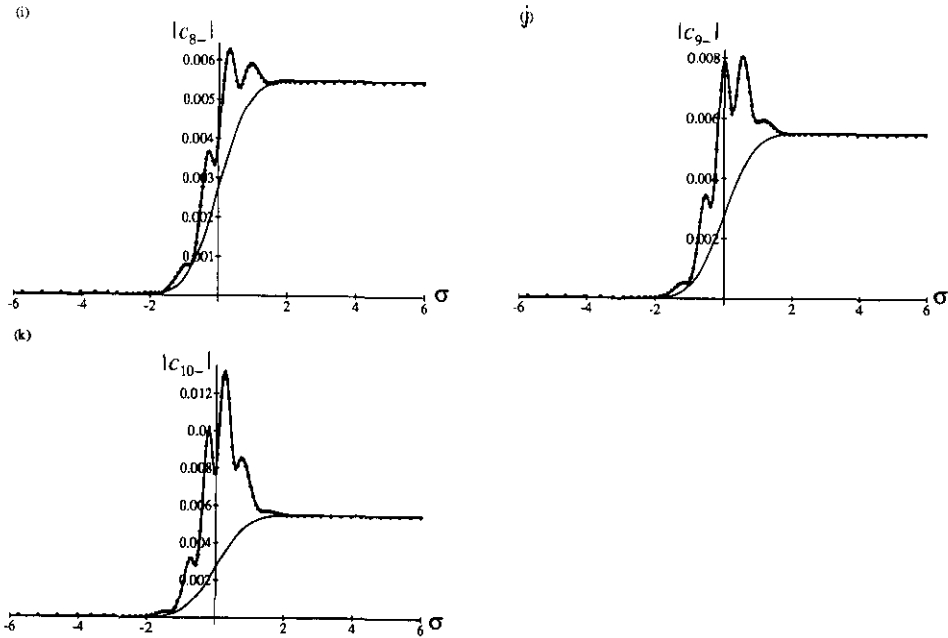


Figure 1. (continued)

The sequence of transition amplitude histories for the two models is shown in figure 1, for the superadiabatic bases  $n = 0$  through  $n = 10$ . Instead of  $\tau$ , we employ the natural variable  $\sigma$  defined in (14), that is we plot  $|c_{n-}(\tau(\sigma))|$ . In the first few bases the two models give markedly different histories: the oscillations differ in amplitude (although they are similar in phase). The gradual attainment of universality as  $n$  approaches 5 is obvious. Not only do the two sets of histories become almost identical, but the amplitude fluctuations get smaller and smoother. For  $n = 4, 5$  and  $6$  the theoretical error function is a good fit to the calculated histories. As  $n$  is further increased beyond optimality, the fluctuations reappear and grow rapidly, reflecting the divergence of the asymptotic series employed to generate the bases.

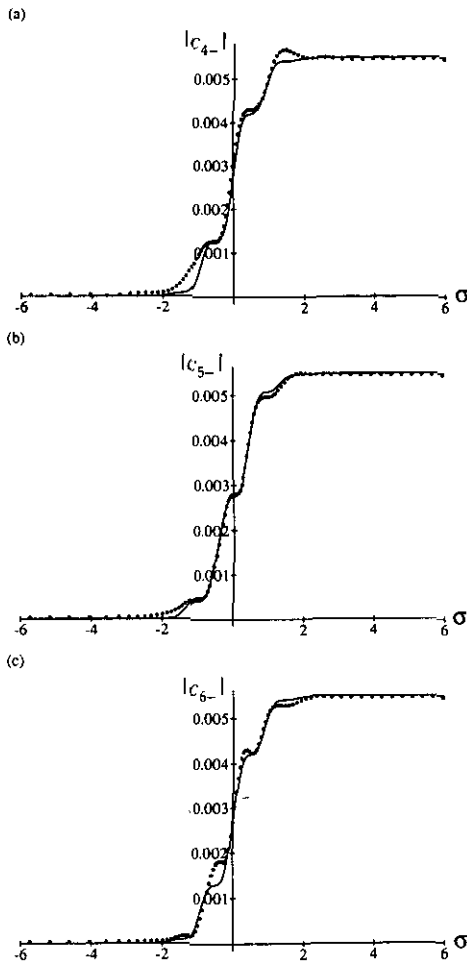
Although the fit with the theoretical formula (14) is good near  $n = 5$ , it is not perfect: the smooth error function is contaminated by small superimposed oscillations. These arise from the discarded second exponential in (13), for which the oscillations in the integrand do not cancel. The corresponding small oscillatory correction to (14), easily estimated by integration by parts, is

$$(-1)^{n+1} \exp\left\{-\frac{|w_c|}{\varepsilon}\right\} \sqrt{\frac{\varepsilon|w_c|}{2\pi}} \exp\left\{-\frac{w^2}{2\varepsilon|w_c|} - \frac{2iw}{\varepsilon}\right\} (w + 2i|w_c|)^{-1}. \quad (23)$$

As figure 2 shows (for the tanh model), the agreement between this ‘improved error function’, and the transition histories close to the optimal one, is strikingly good.

One feature of the optimal history ( $n \sim |w_c|/\varepsilon$ ), emphasized in I, is that it is much more compact than the ordinary adiabatic history ( $n = 0$ ): in the former, the duration of the transition is a time  $\tau_{\text{trans}}$  of order  $\sqrt{\varepsilon}$ , whereas for the latter  $\tau_{\text{trans}}$  is of order unity (essentially the time over which  $\hat{H}(\tau)$  changes), which is considerably longer. In a fixed basis (unrelated to the adiabatic eigenstates),  $\tau_{\text{trans}}$  can be much greater still,



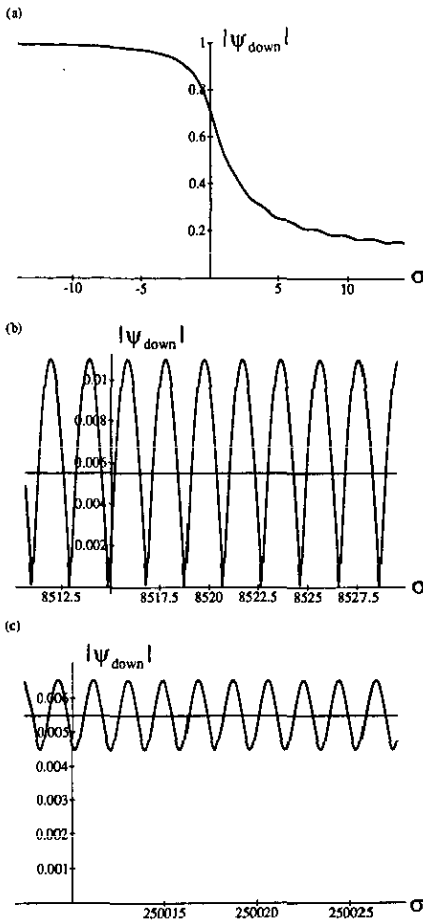


**Figure 2.** (a)-(c). Comparison of the near-optimal transition histories  $|c_{n-}(\sigma)|$  for  $n = 4, 5, 6$ , calculated for the tanh Hamiltonian (dots) with the theory based on the error function (14) with the correction (23) (thin line).

as we now illustrate for the Landau-Zener model. There, a natural representation is the original spin-up, spin-down ('diabatic') basis of equation (1), because the adiabatic state starting in the down state ends in the up state (and vice versa). Figure 3 shows the history of the spin-down Landau-Zener amplitude  $\psi_{\text{down}}$  for the previous value  $\varepsilon = 0.3018$ . The amplitude decays from unity to the final transition amplitude 0.0055. Evidently this decay is accompanied by a long tail of oscillations. Asymptotics of (21), described in appendix A, shows that this tail is exponentially long:  $\tau_{\text{trans}}$  is of order  $\exp(|w_c|/\varepsilon)$ .

## 5. Concluding remarks

The results we have presented not only confirm the predictions of 1 but provide convincing illustrations of recent insights into asymptotics. We have followed the birth,



**Figure 3.** History of the spin-down amplitude  $|\psi_{\text{down}}|$  in the diabatic representation, for the Landau-Zener Hamiltonian, (a) for short times; (b) part of the long-time tail (appendix A) near the time  $\sigma_{\text{trans}} \approx 8517$  when the envelope of the oscillations touches zero; (c) for times where  $\sigma \gg \sigma_{\text{trans}}$ . The thin line is the (exponentially small) final amplitude. Note the difference in  $\sigma$  scales from figures 1 and 2.

across a Stokes line, of the subdominant exponential, for the particular example of a quantum transition, by constructing asymptotic series for the components of an evolving quantum state. By increasing the number of terms used, we were able to witness the progressive attainment of the smooth and universal error function rise corresponding to least-term truncation. Such scrutiny of the Stokes multiplier at each level of asymptotic approximation would barely have been feasible were it not for today's computational software packages, whose increasing prevalence ought to make asymptotics much less of an esoteric pursuit.

One problem that remains to be tackled is that of a Hamiltonian whose complex energy degeneracies are equidistant from the real axis of the  $w$  plane. The contribution of these competing singularities to the final transition amplitude is approximately the interfering sum of complex contributions but when the error functions (Stokes smoothings) overlap, the effect on the transition histories is not entirely clear.

### Appendix A. Landau-Zener asymptotics

From equation (21) we see that the explanation of the oscillations in figure 3 depends on the behaviour of

$$\psi_{\text{down}}(\tau) = \exp\left\{-\frac{\pi}{8\varepsilon}\right\} D_{i/2\varepsilon}\left\{\tau\sqrt{\frac{2}{\varepsilon}}\exp(3\pi i/4)\right\} \quad (\text{A1})$$

for large positive  $\tau$ . In this argument range the parabolic cylinder function asymptotics is based on two exponentials (see e.g. Gradshteyn and Ryzhik 1980, equation 9.246.2), whose mutual interference produces the oscillations. One exponential is larger than the other, by a factor proportional to  $\tau$ , so that the oscillations gradually die away, leaving the ultimate amplitude  $|\psi_{\text{down}}| \rightarrow \exp(-\pi/(2\varepsilon))$ .

To describe these phenomena in lowest order we require the leading term of both exponentials, and a little calculation leads to

$$|\psi_{\text{down}}(\tau)| \xrightarrow{\tau \gg \sqrt{\varepsilon}} \exp\left\{-\frac{\pi}{2\varepsilon}\right\} \left| 1 - \frac{\sqrt{\exp(\pi/\varepsilon) - 1}}{2\tau} \exp\{-i\phi(\tau)\} \right| \quad (\text{A2})$$

where

$$\phi(\tau) \equiv \frac{\tau^2}{\varepsilon} + \frac{1}{\varepsilon} \log\left(\tau\sqrt{\frac{2}{\varepsilon}}\right) + \frac{3\pi}{4} - \arg \Gamma\left(\frac{i}{2\varepsilon}\right).$$

Figure 3(b) illustrates the behaviour of this function. The oscillations lie between two envelopes. The instant when the lower envelope touches zero can be regarded as defining the duration of the transition, i.e.

$$\tau_{\text{trans}} = \frac{1}{2} \sqrt{\exp(\pi/\varepsilon) - 1} \approx \frac{1}{2} \exp(\pi/2\varepsilon). \quad (\text{A3})$$

(At this instant, the period of the oscillations is approximately  $2\pi\varepsilon \exp(-\pi/2\varepsilon)$ .)

In this diabatic basis the transition time is very long. For the value  $\varepsilon = 0.3018$  that we have been using for illustration,  $\tau_{\text{trans}} = 91.07$  and the corresponding Stokes variable is  $\sigma_{\text{trans}} \approx 8517$ . By contrast, the value in the ordinary adiabatic basis is  $\sigma_{\text{trans}} \approx w(1)/\sqrt{\pi\varepsilon} \approx 3$ , and the optimal superadiabatic value is  $\sigma_{\text{trans}} \approx 1$ .

At large negative times,  $|\psi_{\text{down}}|$  approaches its starting value of unity. In this range of argument the parabolic cylinder function has only one exponential contribution (see e.g. Gradshteyn and Ryzhik 1980, equation 9.246.1), so there are no interference oscillations. (Such oscillations appear in a calculation by Berry 1984 but should be disregarded because they are a computational artefact.)

### References

- Berry M V 1984 *J. Phys. A: Math. Gen.* **17** 1225-33  
 — 1989 *Proc. R. Soc. A* **422** 7-21  
 — 1990a *Proc. R. Soc. A* **427** 265-80  
 — 1990b *Proc. R. Soc. A* **429** 61-72 (reference 1 of the text)  
 Dingle R B 1973 *Asymptotic Expansions: Their Derivation and Interpretation* (New York: Academic)  
 Gradshteyn I S and Ryzhik I M 1980 *Table of Integrals, Series and Products* (New York: Academic)  
 Landau L D and Lifshitz E M 1977 *Quantum Mechanics (Non-relativistic Theory)* 3rd edn (London: Pergamon)  
 Zener C 1932 *Proc. R. Soc. A* **317** 696-702