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# Overlapping Stokes smoothings in adiabatic quantum transitions

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**Abstract.** A two-state quantum system whose Hamiltonian varies adiabatically has a weak probability of making transitions between its instantaneous energy eigenstates. If the system is started out in an eigenstate and its evolution tracked using suitably-defined 'superadiabatic' states, the transition probability exhibits the error-function growth characteristic of the birth of subdominant exponentials across Stokes lines. Here we study model Hamiltonians associated with pairs of Stokes lines in the complex time-plane. The overlapping of Stokes crossing phenomena influences the final transition probability and also leads to interference effects in the transition history. These effects can be adjusted by turning parameters in the models.

## 1. Introduction

Weak transitions in a quantum system whose Hamiltonian  $\hat{H}(\tau)$  is adiabatically perturbed provide an excellent illustration of the Stokes phenomenon of asymptotics (Berry 1990a, hereafter called I, and Lim and Berry 1991, hereafter II). For simplicity, we focus on two-level systems and ensure that transitions are weak by requiring that  $\hat{H}(\tau)$  has no degenerate eigenvalues for real  $\tau$ . It is well known (Landau and Lifshitz 1977) that if the system begins in an eigenstate, the transition amplitude (square root of the transition probability) after infinite time is exponentially small in the adiabatic parameter  $\varepsilon$  governing the rate of the perturbation, i.e. the transition amplitude  $\sim \exp(-w_c/\varepsilon)$  where the quantity  $w_c$  will be defined shortly. The weak appearance of the other eigenstate corresponds to the Stokes phenomenon, in which the subdominant partner of two exponentials in an asymptotic expansion appears weakly as a Stokes line is crossed (Berry 1989).

This correspondence arises because exponentials enter into the quantum problem in a way which is natural, yet has subtle consequences. The slowly perturbed system adheres closely not to the instantaneous energy eigenstate, but to this state multiplied by a time-dependent phase factor (complex exponential) which is proportional to the time-integral of the energy eigenvalue. Although such exponentials clearly cannot enter into the transition amplitude, their presence actually underpins the link with the Stokes phenomenon. Studying the transitions using a pair of basis states whose definition includes these phase factors makes it possible to observe refinements in the Stokes phenomenon, such as the optimal error-function smoothing of the growth of the transition amplitude (described in I and depicted in II). The optimal basis is part of a sequence of 'superadiabatic' bases, the procedure for whose construction is outlined in section 2 (and derived fully in I).

Here we go a step beyond II, and study Hamiltonians whose matrix elements are such that the evolution of the quantum system involves the crossing of two Stokes lines. Each Stokes jump is of the same magnitude, but the transition amplitude is not, in general, doubled because the overlapping of the smoothings gives rise to interference effects. These affect both the final transition probability and the history of the transition. The transition history becomes the sum of error functions with a relative phase; their widths and separations can be adjusted by varying parameters in the Hamiltonian.

## 2. Background

### 2.1. Superadiabatic bases

We wish to solve the Schrödinger equation

$$\hat{H}(\tau)|\psi(\tau)\rangle = i\varepsilon \frac{d}{d\tau} |\psi(\tau)\rangle \quad (1)$$

where we can take  $\hat{H}(\tau)$  to be a real symmetric  $2 \times 2$  matrix (analytic in a strip containing the real time-axis)

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

and we have replaced  $\hbar$  with the adiabatic parameter  $\varepsilon$  and scaled time  $\tau$ . (The only generality we lose by taking  $\hat{H}$  real is the exclusion of contributions to the transition probability which are analogous to geometric phases (Berry 1990b, Joye *et al* 1991a); such contributions will not concern us here.) The energy eigenvalues are  $\pm H(\tau) = \pm (Z^2(\tau) + X^2(\tau))^{1/2}$  and we require that  $H(\tau) \neq 0$  for real  $\tau$ .

The system governed by (1) starts out in the upper energy eigenstate at  $\tau = -\infty$ . The aim is to describe the subsequent evolution in terms of transitions between the orthogonal basis states  $|\psi_{n+}(\tau)\rangle$  and  $|\psi_{n-}(\tau)\rangle$ , which are part of a sequence of bases given by expansions in  $\varepsilon$  of order  $n$ . The plus states of all the bases coincide with the actual evolving state as  $\tau \rightarrow -\infty$ , i.e. if we write

$$|\psi(\tau)\rangle = c_{n+}(\tau)|\psi_{n+}(\tau)\rangle + c_{n-}(\tau)|\psi_{n-}(\tau)\rangle \quad (3)$$

we would require that  $c_{n+}(\tau \rightarrow -\infty) = 1$ . To obtain the transition history  $c_{n-}(\tau)$  we need to know the procedure for constructing  $|\psi_{n-}\rangle$ . It is given by

$$|\psi_{n-}(\tau)\rangle = \exp \left[ \frac{i}{\varepsilon} \int_{-\infty}^{\tau} H(\tau') d\tau' \right] \sum_{m=0}^n \varepsilon^m [\alpha_m(\tau) |+(\tau)\rangle - (\tau)\rangle] \quad (4)$$

with

$$|+(\tau)\rangle = \begin{pmatrix} \cos \left[ \frac{\theta(\tau)}{2} \right] \\ \sin \left[ \frac{\theta(\tau)}{2} \right] \end{pmatrix} \quad |-(\tau)\rangle = \begin{pmatrix} \sin \left[ \frac{\theta(\tau)}{2} \right] \\ -\cos \left[ \frac{\theta(\tau)}{2} \right] \end{pmatrix} \quad (5)$$

being the instantaneous energy eigenstates. In accordance with our boundary conditions at  $\tau = -\infty$  the zeroth-order 'adiabatic' basis has  $\alpha_0(\tau) = 0$  and  $\beta_0(\tau) = 1$ . The exponential in (4) is the phase factor mentioned in section 1; the conjugate phase factor occurs in the definition of  $|\psi_{n+}(\tau)\rangle$ .

To construct  $|\psi_{n-}\rangle$ , we solve for  $\alpha_m(\tau)$  and  $\beta_m(\tau)$  by requiring that  $|\psi\rangle = |\psi_{\infty-}\rangle$  formally (see I). This gives the following recursion relations

$$\left. \begin{aligned} \alpha_1(\tau) &= \frac{i\dot{\theta}}{4H} \\ \alpha_{m+1}(\tau) &= \frac{i\dot{\theta}}{2H} \left[ \frac{\dot{\alpha}_m}{\dot{\theta}} + \frac{1}{4} \int_{-\infty}^{\tau} d\tau' \left( \alpha_m(\tau') \frac{d\theta(\tau')}{d\tau'} \right) \right] \\ \beta_{m+1}(\tau) &= \frac{1}{2} \int_{-\infty}^{\tau} d\tau' \left( \alpha_m(\tau') \frac{d\theta(\tau')}{d\tau'} \right) \end{aligned} \right\} \quad m \geq 1. \quad (6)$$

(Similar equations exist for  $|\psi_{n+}(\tau)\rangle$ .) These generate very complicated functions which, in general, can only be obtained by numerical iteration. For certain models, however, they can be found analytically using computer algebra.

Note that in order for the coefficients  $\alpha_m$  and  $\beta_m$  to be finite for large real  $\tau$ , it is sufficient for a Hamiltonian to satisfy  $|\dot{\theta}/H| \rightarrow 0$  as  $|\tau| \rightarrow \infty$  on the real axis. We do not derive this here, but as this condition makes the  $\alpha_m$  go to zero for large positive times, it is not hard to see that it guarantees the  $\beta_m$  remain finite (provided that  $\dot{\theta}$  either stays finite or goes to zero as  $\tau \rightarrow \infty$ , both of which are not unreasonable).

## 2. Transitions and the Stokes phenomenon

We now introduce the monotonically increasing function of time

$$w(\tau) \equiv 2 \int_0^{\tau} H(\tau') d\tau' \quad (7)$$

which will be useful for reparameterizing later results. Along a Stokes line, the ratio of the magnitudes of the exponentials in an asymptotic expansion changes at a maximal rate. Stokes lines are thus like lines of steepest ascent/descent for the exponents. Since the exponents in our pair of basis states are  $\pm iw/2\epsilon$ , the Stokes lines correspond to  $\text{Re } w = \text{constant}$  (so that only  $\text{Im } w$  changes along them). We fix this constant by making the Stokes lines pass through saddle points  $w_c$  of  $w$ , where  $w'(\tau)$  and hence  $H$  are zero; the constant is thus  $\text{Re } w_c$ . Such a choice is natural, for the zeros of  $H$  are branch points around which an asymptotic expansion containing one exponential cannot be analytically continued without introducing the other (Morse and Feshbach 1953).

Thus Stokes lines connect points in the complex  $w$ -plane corresponding to energy degeneracies at complex times. In this general sense, transitions may be regarded as being associated with the energy gap between the states going to zero when  $H(\tau)$  is analytically continued off the real time axis. Note that since the final transition amplitude is exponentially small in  $\epsilon$ , only those values of  $w_c$  closest to the real axis and in the lower half-plane need be considered. Indeed to observe Stokes jumps of comparable magnitude, we require that these points have similar imaginary parts.

However, such complex energy degeneracies are not essential to the existence of transitions. If we rewrite our Schrödinger equation in terms of  $w$ , we have

$$\frac{1}{2} \begin{pmatrix} \cos \theta(w) & \sin \theta(w) \\ \sin \theta(w) & -\cos \theta(w) \end{pmatrix} |\psi(w)\rangle = i\varepsilon \frac{d}{dw} |\psi(w)\rangle \quad (8)$$

which has constant energy eigenvalues. Adiabatic transitions survive, however, because the quantities  $w_c$  are now complex poles of the quantity  $d\theta/dw$  which enters into the perturbation-theory integral giving the transition history (see I):

$$c_{n-}(w) \approx -i(-\varepsilon)^n \int_{-\infty}^w dw' \alpha_{n+1}(w') \exp\left(-\frac{iw'}{\varepsilon}\right). \quad (9)$$

(In what follows, we generally suppress the minus subscript in  $c_{n-}$  as it is understood we are looking at transitions to the lower superadiabatic states.) As can be observed from (6), the  $\alpha_n$  contain successively higher powers of  $d\theta/dw$  by recursion, and use of a theorem due to Darboux (Henrici 1977) shows we may approximate  $\alpha_n$  on the real axis by its singular form near the poles  $w_c$ , provided  $n$  is large. This form gives us a non-vanishing contribution to the integral (9) and may be used to evaluate the transition history, as explained in I and also in Berry and Lim 1993 (hereafter called III).

We obtain the final transition amplitude  $c_n(\infty)$  by deforming the contour of integration below the real axis and around poles of  $d\theta/dw$ , after which we may use the residue theorem. The Stokes phenomenon also survives despite the lack of saddle points, because there is still a Stokes line at  $\text{Re } w = 0$ . To observe error-function smoothing of the Stokes jump, we use (4) up to its least term, i.e. at  $n \sim |\text{Im}(w_c)|/\varepsilon$  (see I). Then the smoothing we obtain for each pole  $w_c$  is, with  $r = |\text{Re } w_c|$  and  $s = |\text{Im } w_c|$ .

$$c_n(w) \approx \exp\left(-\frac{s+ir}{\varepsilon}\right) \times \left\{ \frac{1}{2} \left[ 1 + \text{erf}\left(\frac{w-r}{\sqrt{2\varepsilon s}}\right) \right] + \frac{(-1)^{n+1}}{w-r+2s} \sqrt{\frac{\varepsilon s}{2\pi}} \exp\left[-\frac{(w-r)^2}{2\varepsilon s} - \frac{2iw}{\varepsilon} + \frac{2ir}{\varepsilon}\right] \right\}. \quad (10)$$

(The exponential term in the curly brackets describes small oscillations in the smoothing. These are calculated and displayed in II but we do not use them here.)

In the more general case where we have several poles  $m$  of comparable proximity to the real axis, it is plausible to just add contributions of the form given by (10), with the important caveat that we must consider the signs of the residues at these poles. These are not independent of one another, as we discuss in the next section. The final transition amplitude, for example, is

$$c_n(\infty) = \sum_m (\pm)_m \exp\left(-\frac{s_m+ir_m}{\varepsilon}\right) \quad (11)$$

where the  $(\pm)_m$  denotes the appropriate sign for the residue at the  $m$ th pole. This is derived and discussed in considerable detail by Joye *et al* (1991b). (In fact (10), and hence (11), can contain an additional and non-trivial prefactor for certain models, a fact we discuss in III.)

As a basic example, take the well-known Landau-Zener Hamiltonian (Zener 1932). This has  $Z = \tau$ ,  $X = 1$ . It has energy degeneracies at  $w_c = \pm i\pi/2$ , i.e. the Stokes line is the imaginary axis in the  $w$ -plane, which is crossed at  $w = \tau = 0$ . The optimal transition

history is indeed an error function centred on  $w=0$ , with the expected width and height (figure 1 of II). For more complicated models with overlapping smoothings, one might expect to see some merging of the error functions as well as interference resulting from error functions switching on with different phases. We shall demonstrate that this is indeed what is observed.

### 3. Demkov–Kunike model

Now consider a Hamiltonian due to Demkov and Kunike (1969), recently studied by Suominen and Garraway (1992):

$$Z(\tau) = \tanh \tau \quad X(\tau) = \sqrt{a^2 + 1} \operatorname{sech} \tau \tag{12}$$

where  $a$  is a real parameter. This model, which is exactly solvable, has energy degeneracies at times  $\tau_c$  given by  $Z(\tau_c) = \pm iX(\tau_c)$ , i.e.

$$\tau_c = \pm \sinh^{-1}(i\sqrt{a^2 + 1}). \tag{13}$$

These correspond to (Suominen and Garraway 1992), with  $n$  integral

$$w_c = \pi[a + i(4n \pm 1)] \tag{14}$$

and also to the reflections of these points in the line  $\operatorname{Re} w_c = 0$  (figure 1). Near these points (see appendix B of I), and with the restriction that  $a \neq 0$ ,

$$\frac{d\theta}{dw} = \pm \frac{i}{3(w - w_c)}. \tag{15}$$

What is important to note is that the  $\pm$  signs in (15) are matched to those in (13), i.e. pairs of points on the same side of the real axis in the  $w$ -plane have the same sign in the numerator of (15). Therefore when we deform the contour of integration in (9)

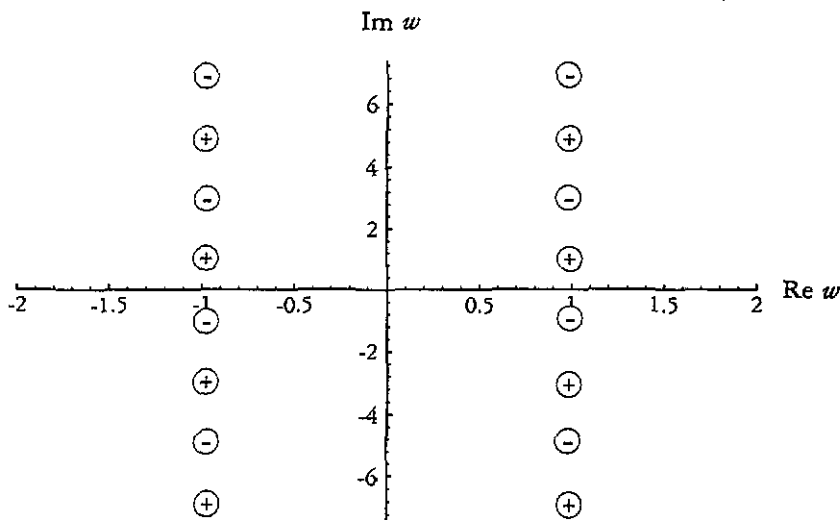


Figure 1. Singularities of  $w_c$  of  $d\theta/dw$  for the Demkov–Kunike model with  $a=1$ . Each circle is centred on a singularity and contains the sign of the residue at that point. The axes are labelled in units of  $\pi$ .

around such pairs, the residues from each pole have the same sign. Since the contribution of the nearest pair to the real axis dominates over the others for small  $\varepsilon$ , the final transition amplitude is given by (11) as

$$|c_n(\infty)| = 2 \cos \frac{\pi a}{\varepsilon} \exp\left(-\frac{\pi}{\varepsilon}\right). \quad (16)$$

This is borne out by examining the analytical solution of the Schrödinger equation (Suominen and Garraway 1992). Note that it is not difficult to find models where residues from pairs of poles have opposite signs; an example is  $Z = \tau^2$ ,  $X = 1$  (Suominen 1992).

The recursion relations (6) for the Demkov-Kunike model can also be exactly solved using symbolic packages. A practical way is to rewrite (6) in terms of  $\theta$ , then use

$$\frac{d\theta}{dw} = -\frac{1}{8(a^2+1)} [(a^2+4) \sin \theta + a^2 \cos 3\theta]. \quad (17)$$

The case  $a=0$  is an example of the situation discussed earlier, where the energy levels become constant ( $= \pm 1$ ) but transitions still occur because the points  $w_c$  are now poles of  $d\theta/dw$ . Since the pair of poles nearest the real axis has now coalesced to one point, we might expect (16) to be incorrect and that the prefactor of 2 should become 1. In fact (16) remains valid because the residue has changed accordingly (this is the non-trivial prefactor discussed in III and also Joye 1993). The transition histories one obtains look very like those for Landau-Zener, and hence we do not include them here.

Equations (10) and (16) make clear that one cannot hope to independently adjust the final transition probability and the placement and width of the optimal error functions, since changes in  $a$  would affect all of these. The order at which optimality is obtained is also affected. For our purposes, we have initially chosen to keep the final transition amplitude constant at zero (by making the cosine in (16) zero) while changing  $a$  and  $\varepsilon$  to cause the gradual coalescence of the Stokes smoothings. With  $a=2$  and  $\varepsilon = \frac{4}{3}$ , the error functions are widely separated. Figure 2 shows the sequence of transition histories with the optimal order at 7. Note that the error functions are centred at the correct locations and show the same small oscillations that one can observe and account for in the Landau-Zener model (ii). In figure 3, for  $a = \frac{1}{4}$ ,  $\varepsilon = \frac{1}{2}$ , the error functions have merged together.

In the above cases, the Stokes jumps are out of phase by  $\pi$ , and it appears as though the transition switches on and then off again. However, if we make the cosine in (16) equal to  $\pm \frac{1}{2}$ , we might expect the second error function to be somewhat suppressed since the final transition amplitude is equal to the height of the first error function. This is indeed what we see, as illustrated in figure 4 for the case  $a=1$ ,  $\varepsilon = \frac{3}{7}$ .

It is not obvious that the second error function can be retrieved, but we can do this using the fact that the error functions are out of phase by  $14\pi/3$  radians (effectively  $120^\circ$ ). Hence if we wish to see both error functions contributing equally to the final transition history, we calculate the component of  $c_n$  at a phase angle halfway between the two. According to (10), this phase should be zero, with the error functions having phases of  $\pm 60^\circ$ . In fact an additional phase correction  $e^{2i\varphi(a, \varepsilon)}$  is required to achieve this, for reasons given in the appendix. With this correction the two constituent error functions in the optimal history are revealed, as shown in figure 5.

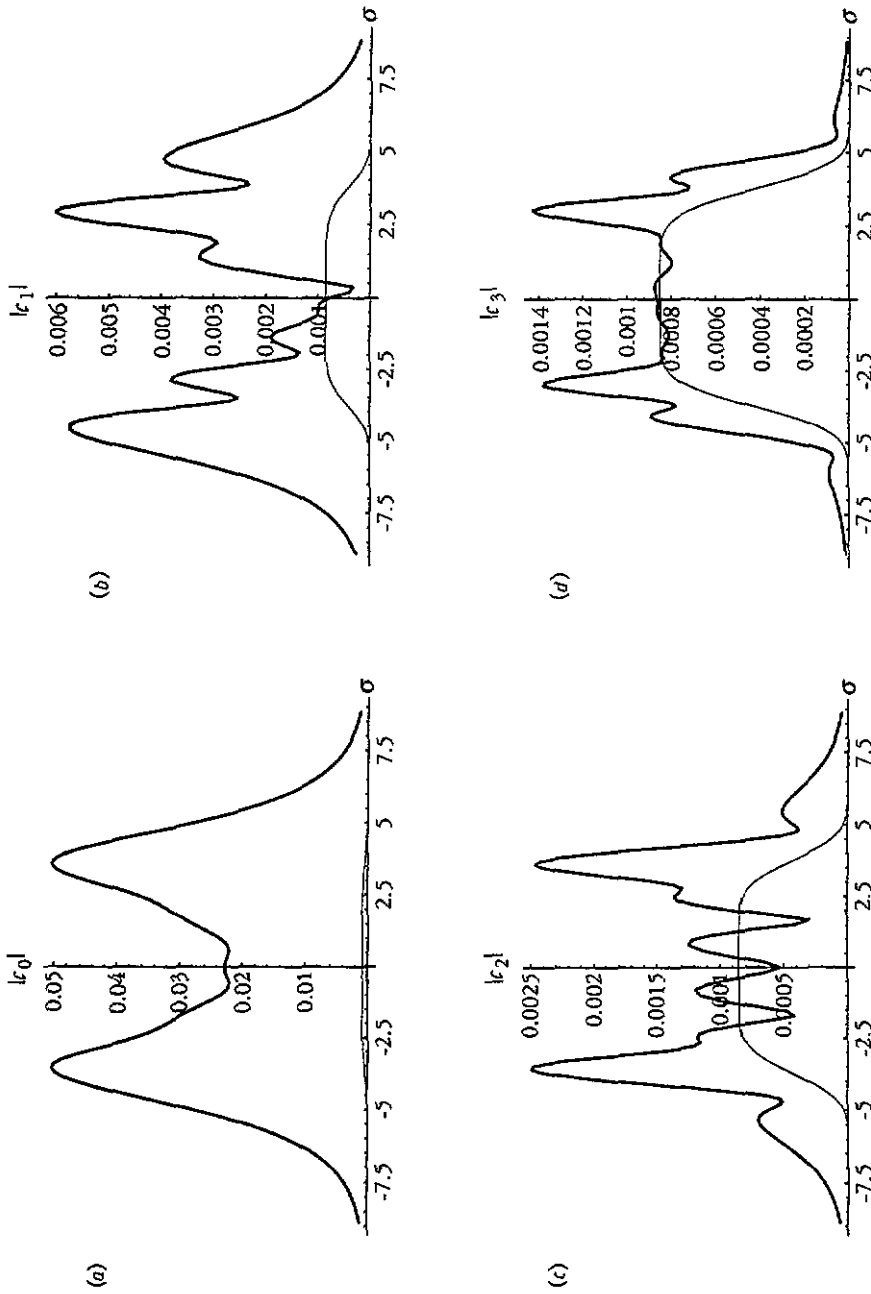


Figure 2. Transition histories for the Demkov-Kunike model with  $\alpha = 2$  and  $\epsilon = \frac{1}{2}$ . The thick lines are the transition amplitudes while the thin line is the optimal history showing well-separated error functions; the quantity  $\sigma \equiv w/\sqrt{2\epsilon}|\text{Im } w_c|$ . The sequence begins with the adiabatic basis, with optimality at  $n=7$ . Note that the error functions are centred on the Stokes lines at  $\sigma = \pm |\text{Re } w_c|/\sqrt{2\epsilon}|\text{Im } w_c| = \pm a\sqrt{\pi/2\epsilon} \approx \pm 3.8$ .



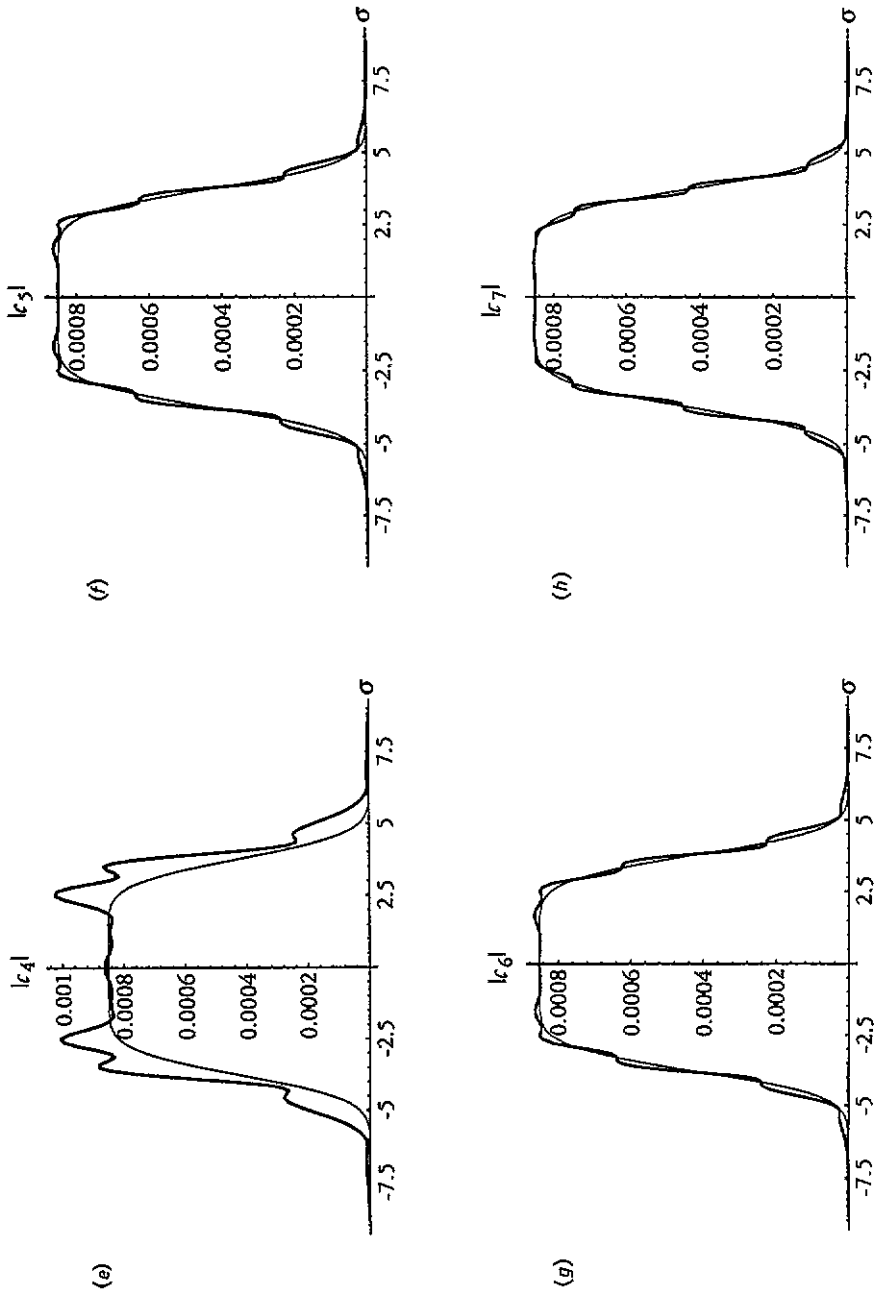


Figure 2. (continued).



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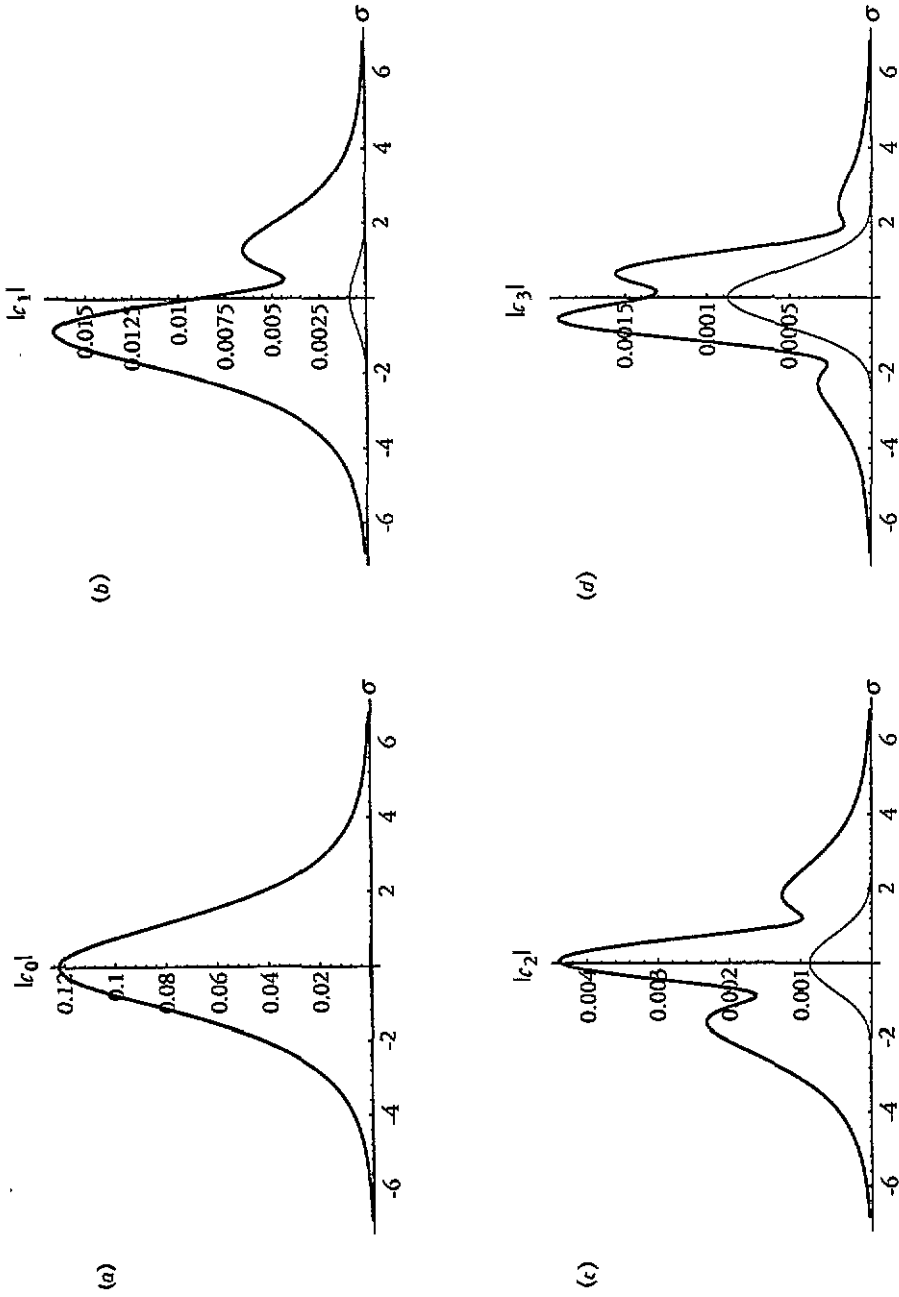


Figure 3. Demkov-Kunike transition histories with  $a = \frac{1}{4}$ ,  $\varepsilon = \frac{1}{2}$ . The error functions at  $\sigma = \sqrt{\pi}/4$  have become merged together and hence one can no longer discern a central plateau.

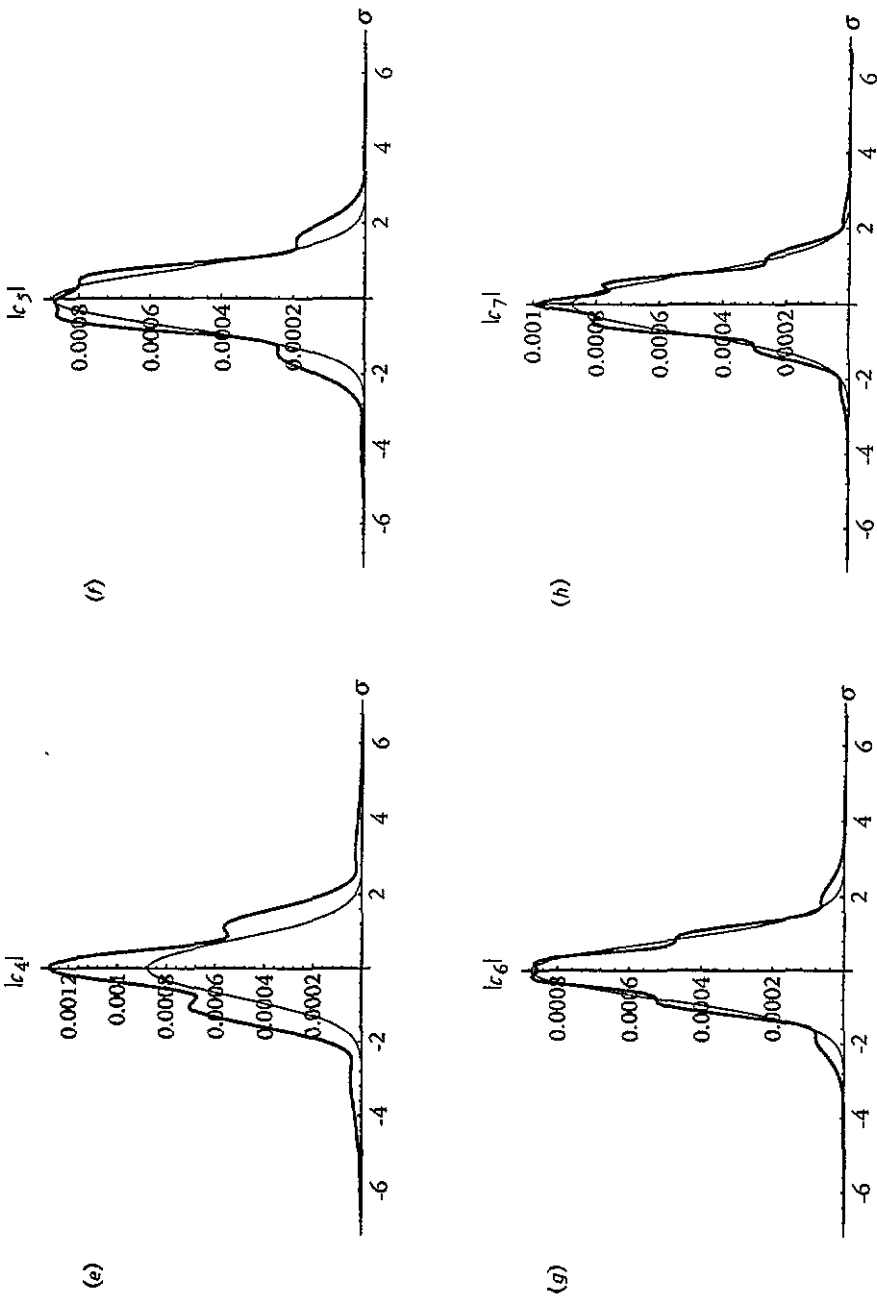


Figure 3. (continued).

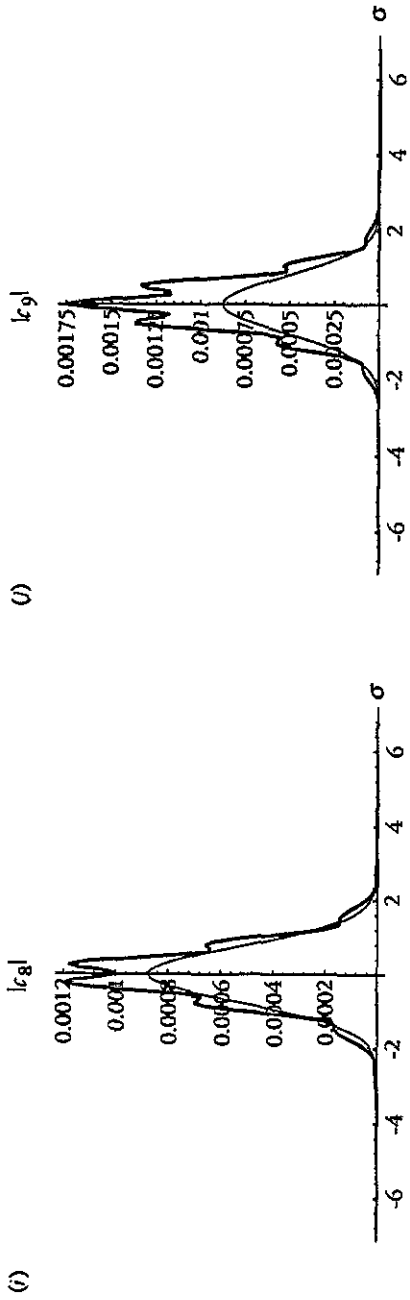


Figure 3. (continued).

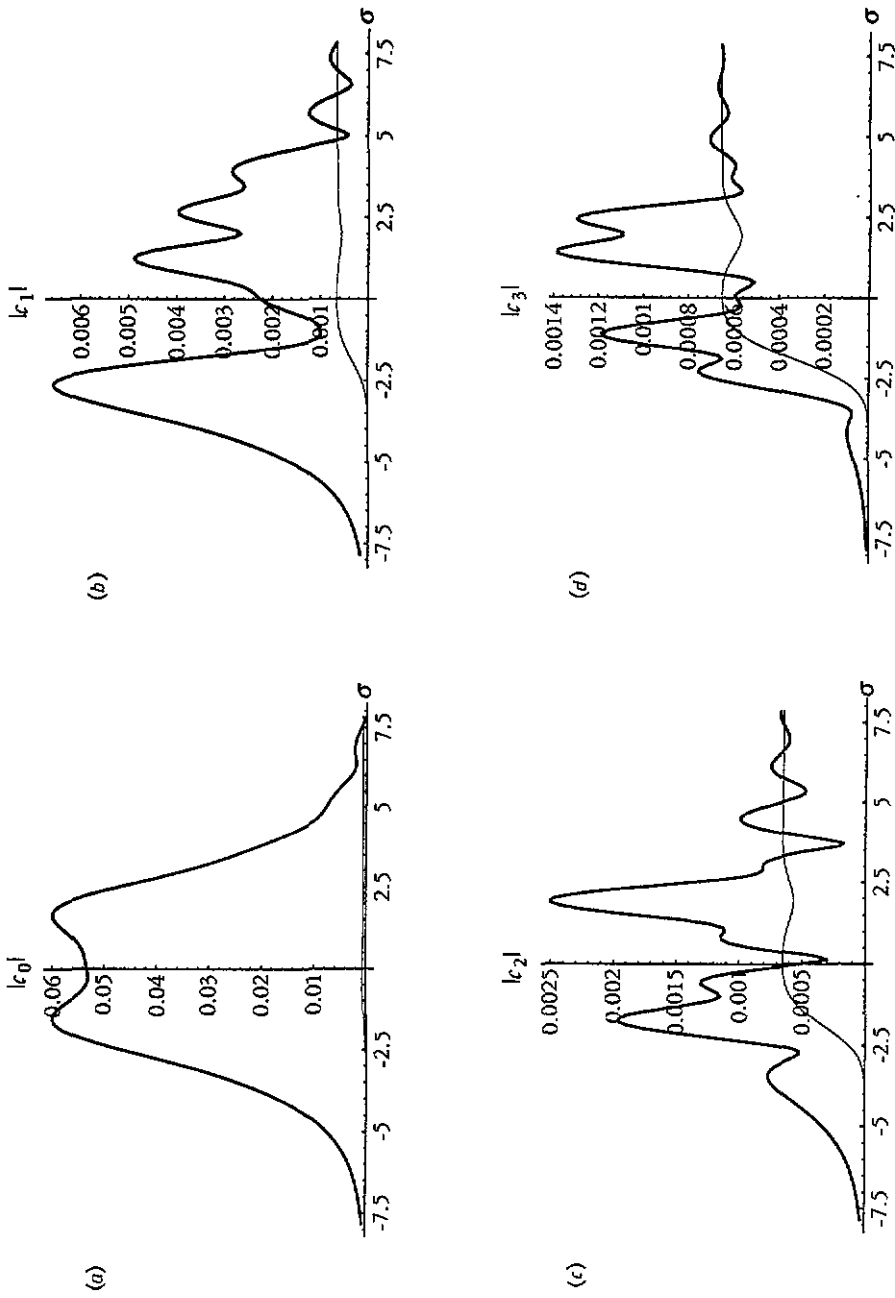


Figure 4. Demkov-Kunike transition histories for  $\alpha=1$ ,  $\epsilon=\frac{1}{7}$ . The second error function is not directly visible because the height of the first equals the final transition amplitude.

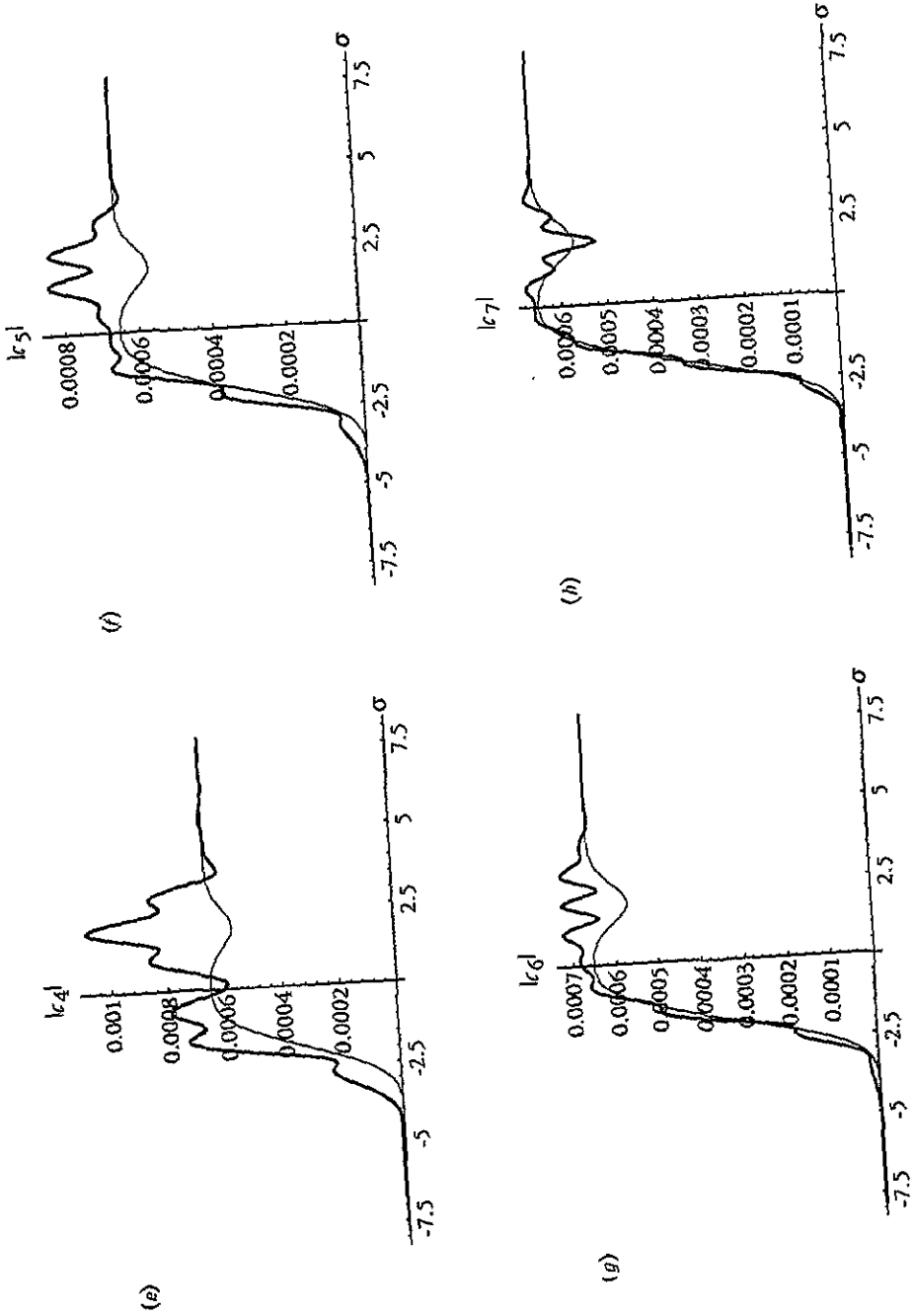


Figure 4. (continued).

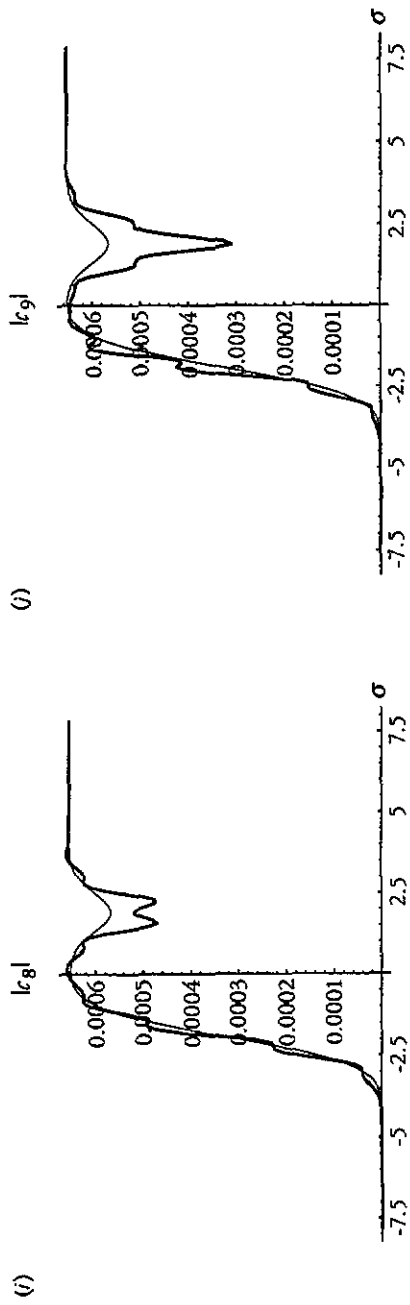


Figure 4. (continued).



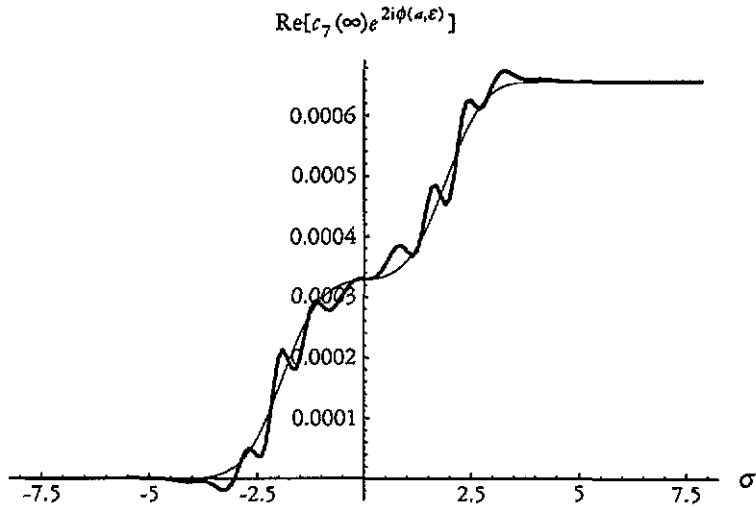


Figure 5. Demkov-Kunike transition history of figure 4, but calculated at a phase midway between those of the two error functions, each of which is now seen to contribute equally to the final result.

#### 4. The modified Landau-Zener model

This Hamiltonian was also studied by Suominen *et al* (1991), who call it 'simple Lorentzian singularity'; it is:

$$Z(\tau) = \frac{\tau}{\sqrt{1+\tau^2}} \quad X(\tau) = \frac{a}{\sqrt{1+\tau^2}} \quad (18)$$

This is like the Landau-Zener model except that the energy levels are finite as  $\tau \rightarrow \pm \infty$ . Energy degeneracies occur at  $\tau = \pm ia$ , and the levels also have a singularity at  $\tau = i$ . For this model,  $w$  is an elliptic integral of the second kind (Gradshteyn and Ryzhik 1980)

$$w(\tau) = 2 \int_0^\tau d\tau' \left[ \frac{\tau'^2 + a^2}{\tau'^2 + 1} \right]^{1/2} = -2iaE \left( i \sinh^{-1}(\tau), \frac{1}{a} \right) \quad (19)$$

and we choose  $w$  to have branch cuts from  $\tau = \pm ia$  ( $a < 1$ ) or  $i$  ( $a > 1$ , figure 6(a)) to  $\pm i\infty$ . We do not know of an analytical solution for this model, nor can the recursion relations (6) be algebraically integrated (except when  $a = 1$ ). Hence we shall confine most of our discussion to the final transition amplitude, which can be computed by solving the Schrödinger equation in the adiabatic basis using the Runge-Kutta method.

There are three cases that need be considered. When  $a < 1$ , there is one energy degeneracy (and its complex conjugate); the pole is further from the real axis than the degeneracy and hence we expect the transition amplitude to be determined from the degeneracy in the usual way. When  $a = 1$ , the energy levels are everywhere constant ( $= \pm 1$ ) but once again there are transitions due to singularities of  $d\theta/dw$  at  $w_c = \pm 2i$ . The residue at these points is such that the (single) exponential in the transition amplitude is multiplied by a prefactor of  $\sqrt{2}$  (III and Joye 1993).

The situation becomes more involved when  $a > 1$  and the degeneracy is further away from the real time-axis than the pole. In the  $w$ -plane, the pole is a complete elliptic

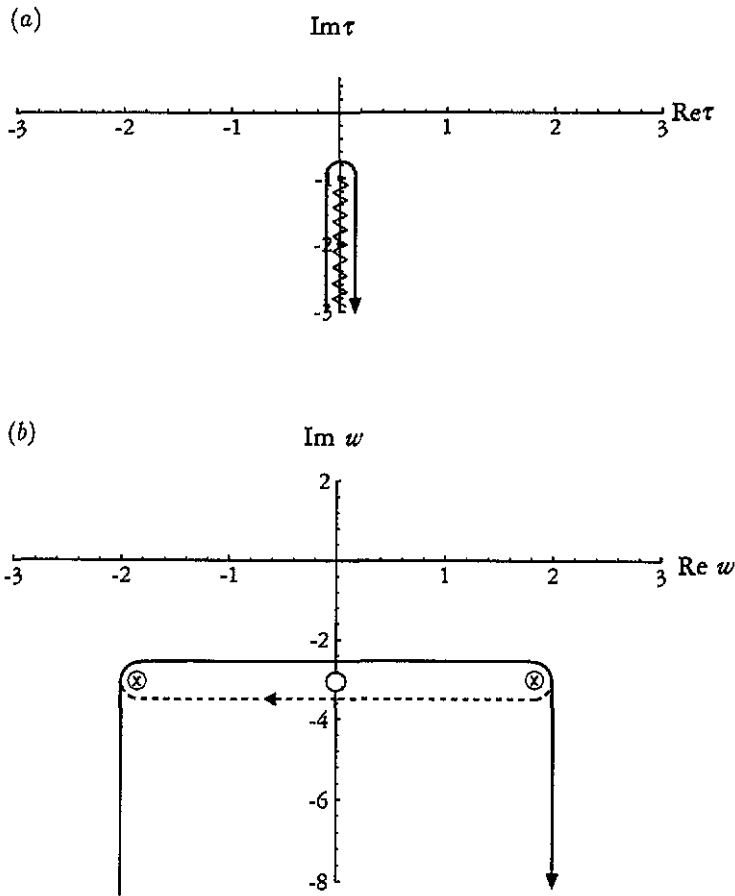


Figure 6. Branch cuts and contours for the transition history integral for the modified Landau-Zener model with  $a=2$ . We have used first-order perturbation theory applied to the adiabatic basis. The contour in the  $\tau$ -plane (a) corresponds to the solid line in the  $w$ -plane (b), which in the absence of branch cuts can be deformed into a loop, the lower part of which is indicated by the dashed line. The crossed circles are energy degeneracies and the unfilled circle is a pole of  $H(\tau)$ .

integral of the second kind  $-2iaE(1/a^2)$ , a pure imaginary quantity, while the degeneracy can be mapped onto two points

$$w_c = \pm 2 \int_1^a dy \left( \frac{a^2 - y^2}{y^2 - 1} \right)^{1/2} - 2iaE \left( \frac{1}{a^2} \right) \tag{20}$$

corresponding to opposite sides of the imaginary axis in the time-plane (figure 6(a), (b)). To obtain the final transition amplitude  $c_n(w \rightarrow \infty)$ , we need to know how the degeneracies and poles affect the evaluation of (9). We do not have explicit forms for the functions  $\alpha_n(w)$  except for the adiabatic basis  $n=0$ , when (see (6) and (9))

$$c_0(w \rightarrow \infty) = \int_{-\infty}^{\infty} dw \frac{d\theta}{dw} \exp\left(-\frac{iw}{\varepsilon}\right) \tag{21}$$

with, written as a function of  $\tau$ ,

$$\frac{d\theta}{dw} = -\frac{a(\tau^2 + 1)^{1/2}}{2(\tau^2 + a^2)^{3/2}} \quad (22)$$

Near the degeneracies  $w_c$ , the behaviour of  $d\theta/dw$  is given by (15) for the Demkov-Kunike model as both models have the same leading-order singularities in their matrix elements (III contains a detailed discussion of this point). Both values of  $w_c$  also have residues with the same sign because they both stem from the same point in the  $\tau$ -plane. Near the pole  $w_i \equiv w(-i)$ , a local expansion of  $d\theta/dw$  and reverting the series shows that

$$\frac{d\theta}{dw} \approx \frac{ia(w - w_i)}{4(a^2 - 1)^2} \quad (23)$$

so that we have a first-order zero which does not contribute to the integral.

We evaluate the integral by deforming the contour off the real  $w$ -axis. Simply converting (21) to a time integral shows that a suitable contour in the  $T$ -plane is one which curls tightly round the pole at  $\tau = -i$  and the branch cut arising from  $w(\tau)$  (figure 6(a)). The corresponding contour in the  $w$ -plane is shown in figure 6(b), which in the absence of branch points can be deformed into the loop passing around  $w_i$  and the two points  $w_c$ . The integral is then given by summing residues at the degeneracies. In fact the answer thus obtained is too large by a factor of  $\pi/3$ , but as explained in I and III this renormalizes in a predictable way to 1. The final transition amplitude is thus expected to be

$$2 \cos \left( \frac{2}{\varepsilon} \int_1^a dy \left( \frac{a^2 - y^2}{y^2 - 1} \right)^{1/2} \right) \exp \left( -\frac{2a}{\varepsilon} E \left( \frac{1}{a^2} \right) \right) \quad a > 1. \quad (24)$$

This is demonstrated in figure 7 for the case  $a=4$ . We have divided out the small exponential from the modulus of the final transition amplitude in order to bring out

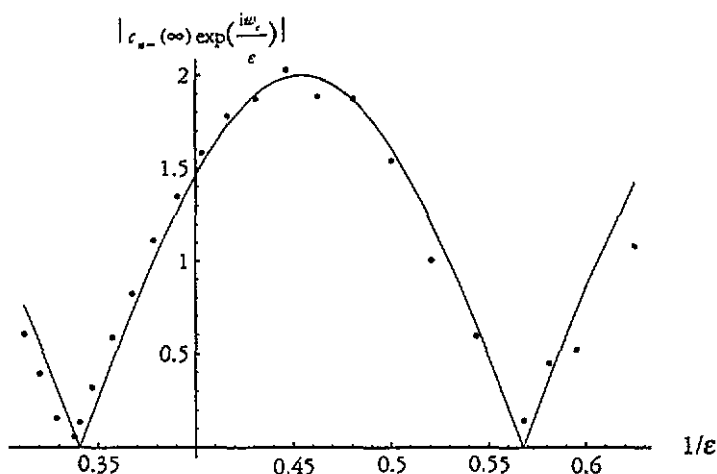


Figure 7. Final transition amplitude (dots) compared with theory (thin line) for the modified Landau-Zener model with  $a=4$ . To highlight the oscillatory behaviour the results have been scaled by dividing out the small exponential.

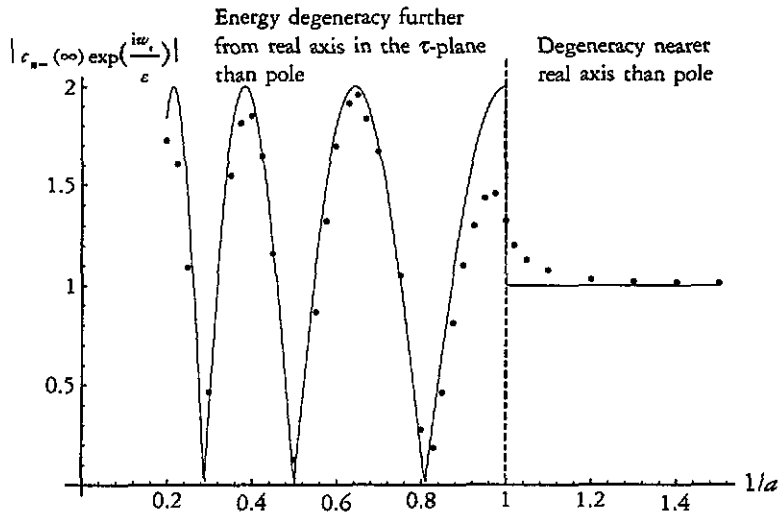


Figure 8. Final transition amplitudes (dots) compared with theory (thin line) for the modified Landau-Zener model with  $\epsilon = 1.6$ ; the results have been scaled by dividing out the small exponential. Note the smooth transition between the two regimes where the degeneracy is nearer/further than the pole from the real axis in the time-plane. In contrast the theoretical result has a discontinuity at  $a = 1$ , for which the transition amplitude is  $\sqrt{2}$ .

the cosinusoidal behaviour (dotted line) over a range of values of  $\epsilon$ . While agreement with theory (solid line) is not perfect, the cosine oscillations can be clearly seen.

The fact that we have only partial agreement with theory, at least as far as the magnitudes of the transition amplitudes are concerned, suggests that there are residual higher-order  $\epsilon$ -corrections from the pole which we have not taken into account. We can attempt to estimate their influence as the separation between pole and degeneracy is varied, with  $\epsilon$  held constant. Figure 8 shows the transition amplitude plotted as a function of  $a$ , with  $\epsilon = 1.6$ . We have again divided out the exponential to show the variation on a scale of unity. It can be seen that agreement with theory is good when  $a$  is not close to 1, i.e. when the degeneracy in the complex time-plane is far from the pole. For  $a \sim 1$ , we see a smooth transition from the regime where there is only one contributing degeneracy ( $a < 1$ ) to the special case  $a = 1$  where we have one degeneracy and a prefactor of  $\sqrt{2}$ , to the regime in which there are two degeneracies ( $a > 1$ ).

## 5. Conclusions

Our results show that adiabatic quantum transitions can be used to provide a remarkably clear and simple illustration of the Stokes phenomenon, especially when more than one Stokes crossing is involved. It is not easy to find such explicit demonstrations of interference between Stokes smoothings in more traditional applications of asymptotics (Berry and Howls 1993).

An obvious remaining area of uncertainty is the lack of precise agreement in cases where the energy degeneracy is further from the real axis in the time-plane than a pole. Our results for the modified Landau-Zener model show the oscillations in the final transition amplitude convincingly, but the agreement is often poor when the results are taken pointwise. It would seem that there is a slight phase shift in the oscillations which

could account for these discrepancies, but we do not as yet have an explanation for such a shift if indeed one exists. The reason for the smooth transition between regimes as the degeneracy moves relative to the pole is also not properly understood. A proper treatment would involve considering corrections which are of higher orders in  $\varepsilon$ , but the correct way to do this is not obvious.

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### Appendix. Behaviour of the Demkov–Kunike model as $\tau \rightarrow \pm \infty$

The exact solution to the Schrödinger equation for the Demkov–Kunike model is derived in several sources, such as Suominen and Garraway (1992). With

$$|\psi(\tau)\rangle \equiv \begin{pmatrix} C_1(\tau) \\ C_2(\tau) \end{pmatrix}$$

the solution can be stated in the form

$$\begin{aligned} C_1 &= \frac{i\varepsilon\alpha\beta e^{i\phi}}{\gamma\sqrt{a^2+b^2}} \left(\frac{\operatorname{sech} \tau}{2}\right)^{1-1/\varepsilon} {}_2F_1(\alpha+1, \beta+1, \gamma+1, \zeta(\tau)) \\ C_2 &= \exp(i\phi) \left(\frac{\operatorname{sech} \tau}{2}\right)^{-i/\varepsilon} {}_2F_1(\alpha, \beta, \gamma, \zeta(\tau)) \end{aligned} \quad (\text{A1})$$

where  ${}_2F_1$  is the hypergeometric function, and

$$\alpha = \frac{a-i}{\varepsilon} \quad \beta = -\frac{a+i}{\varepsilon} \quad \gamma = \frac{1}{2} - \frac{i}{\varepsilon} \quad \zeta(\tau) = \frac{1}{2}(1 + \tanh \tau) \quad (\text{A2})$$

in order to satisfy the boundary condition  $|C_2(\tau \rightarrow -\infty)| = 0$ . The phase factor  $e^{i\phi}$  in (A1) is necessary to ensure that  $c_{n+}(\tau \rightarrow -\infty) = 1$  for all  $n$ . It is determined by matching the terms in (4), using

$$\lim_{\tau \rightarrow \pm \infty} \left(\frac{\operatorname{sech} \tau}{2}\right)^{-i/\varepsilon} {}_2F_1(\alpha, \beta, \gamma, \zeta(\tau)) = |{}_2F_1(\alpha, \beta, \gamma, \zeta(\tau))| \exp\left(\frac{i|\tau|}{\varepsilon}\right) \quad (\text{A3})$$

$$w(\tau) = 2 \left[ \sinh^{-1} \left( \frac{\sinh \tau}{\sqrt{a^2+1}} \right) + a \sin^{-1} \left( \frac{a \tanh \tau}{\sqrt{a^2+1}} \right) \right] \quad (\text{A4})$$

and

$$\lim_{\tau \rightarrow \pm \infty} \exp\left(-\frac{iw(\tau)}{2\varepsilon}\right) = \exp[\mp(i|\tau|/\varepsilon + i\phi)]$$

where

$$\varphi(a, \varepsilon) = \frac{a}{\varepsilon} \sin^{-1} \left( \frac{a}{\sqrt{a^2 + 1}} \right) - \frac{i}{\varepsilon} \log(\sqrt{a^2 + 1}). \quad (\text{A5})$$

This explains the presence of the phases  $e^{i\varphi}$  in (A1). Now note that  $c_{n-}(\tau \rightarrow \infty)$  is  $\langle -|\psi\rangle \exp(-i\omega/2\varepsilon)$  in any basis  $n$ . Use of (A3) and (A4) shows that this complex quantity has argument  $2\varphi(a, \varepsilon)$ . This is the origin of the phase correction mentioned at the end of section 3.

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