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Histories of adiabatic quantum transitions

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The way in which the transition amplitude to an initially unoccupied state increases to its exponentially small final value is studied in detail in the adiabatic approximation, for a 2-state quantum system. By transforming to a series of superadiabatic bases, clinging ever closer to the exact evolving state, it is shown that transition histories renormalize onto a universal one, in which the amplitude grows to its final value as an error function (rather than via large oscillations as in the ordinary adiabatic basis). The time for the universal transition is of order $\sqrt{(\hbar/\delta)}$ where δ is the small adiabatic (slowness) parameter. In perturbation theory the pre-exponential factor of the final amplitude renormalizes superadiabatically from the incorrect value $\frac{1}{3}\pi$ (for the ordinary adiabatic basis) to the correct value unity. The various histories could be observed in spin experiments.

1. Introduction

An adiabatic quantum transition is a transition between two eigenstates of a hamiltonian $\hat{H}$ that varies slowly in time. Such transitions are extremely weak. Indeed, in the limit of infinitely slow change they do not occur at all, because of the adiabatic theorem (Born & Fock 1928; see also Messiah 1962) which guarantees that evolving states cling to the instantaneous eigenstates of $\hat{H}$. As is well known (Dykhne 1962; Davis & Pechukas 1976; Hwang & Pechukas 1977), the amplitude for a transition to occur over infinite time vanishes as $\exp(-1/\delta)$ where δ is the small adiabatic parameter, when (as we assume here) $\hat{H}$ is an analytic function of time in a strip including the real axis.

The usual aim of adiabatic theory is to calculate the probability that a transition has occurred after infinite time. Here the purpose is different: to determine the whole course of the transition, that is, the populations of the states as a function of time. The main result I wish to report is that there exists a natural basis in which the transition occurs in a way that is universal (that is, independent of the detailed time dependence of $\hat{H}$). The amplitude for being in the original unoccupied state is real, and its increase to its final exponentially small value is described by the error function of a natural variable.

Our natural basis is not the usual adiabatic basis, of eigenstates of the instantaneous $\hat{H}$. Rather, it is one of a sequence of *superadiabatic* bases, clinging closely to the actual evolving state, with errors given by successively increasing powers of δ. (Kruskal (1962) made similar transformations in a classical context, and established that the final non-adiabatic transition amplitude is zero to all orders in δ.) The formal transformation to the superadiabatic bases is given in §2, and their actual construction is given in §3. For bases low in the sequence (such as the zero-order usual adiabatic basis), the transition history depends on the details of the time-dependence of $\hat{H}$. Universality emerges when we go to bases high in the sequence, for reasons explained in §4, and leading in §5 to the universal transition history.

A by-product of the work is a new solution, in §6, of the '$\frac{1}{3}\pi$ problem'. This arises because of the technique used to calculate the amplitudes in the various bases, namely lowest-order perturbation theory. When applied to the zero-order (adiabatic) basis, this is well known (Berry & Mount 1972) to yield a final amplitude differing from the exact adiabatic limit by a factor $\frac{1}{3}\pi$. Corrections from higher orders in perturbation theory turn $\frac{1}{3}\pi$ into unity, as shown by Davis & Pechukas (1976) and (with another technique) by Berry (1982). Here $\frac{1}{3}\pi$ renormalizes onto unity in a quite different way, namely by using lowest-order perturbation theory but in successive superadiabatic bases.

It is not surprising (although perhaps unfamiliar) that slightly different bases give very different transition histories. After all, the history must depend on what states the transition is regarded as connecting, and since the final outcome is of order $\exp(-1/\delta)$ its course can be expected to be sensitive to alterations in the basis by powers of δ. But the basis-dependence of the history raises a physical question: could the histories, including the simple universal one, be observed? The answer is that they could, by means of spin experiments explained in §7.

One motivation for this work is renewed interest in the time it takes to make a quantum transition (see Mullen *et al.* 1989 and references therein). Another motivation is recent progress in understanding the detailed asymptotics of functions near Stokes lines, where small exponentials appear and disappear (Berry 1989*a*, *b*; Olver 1990; Jones 1990; Boyd 1990). Formally, the present work is a special case of this, and indeed my recent study (Berry 1990*a*) of the WKB problem from this point of view can be adapted to deal with the adiabatic problem.

2. Transformations to new bases

We wish to understand the solutions $|\psi\rangle$ of Schrödinger's equation

$$\mathrm{i}\hbar\, \mathrm{d}_t|\psi\rangle = \hat{H}(\delta t)\,|\psi\rangle \tag{1}$$

in the adiabatic limit of small δ. The first step is to transform to a new 'slow time' variable τ and new parameter ϵ, defined by

$$\tau \equiv \delta t, \quad \epsilon \equiv \hbar\delta. \tag{2}$$

Thus

$$\mathrm{i}\epsilon|\dot{\psi}(\tau)\rangle = \hat{H}(\tau)\,|\psi(\tau)\rangle, \tag{3}$$

where here and hereafter an overdot denotes a τ derivative.

To study the transition dynamics in detail we restrict ourselves to the simplest model, in which the quantum system has two states:

$$|\psi\rangle = \begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}, \quad \hat{H} = \begin{bmatrix} Z & X \\ X & -Z\end{bmatrix} \equiv H\begin{bmatrix}\cos\theta & \sin\theta \\ \sin\theta & -\cos\theta\end{bmatrix} \tag{4}$$

(all quantities are functions of τ). A familiar special case is the Landau–Zener hamiltonian (Zener 1932), for which X is constant and $Z = \tau$. As explained in Appendix A, there is no loss of generality in choosing $\hat{H}$ traceless, and real symmetric rather than complex hermitian (although the removal of any imaginary part of $\hat{H}$ reveals an interesting geometric phenomenon which I discuss elsewhere (Berry 1990*b*)). It is helpful to think of X, Z as components of a vector $\boldsymbol{H}(\tau)$ in 'hamiltonian space'. As τ increases from $-\infty$ to $+\infty$, $\boldsymbol{H}(\tau)$ draws a curve in hamiltonian space, on whose geometry the evolution of $|\psi\rangle$ depends.

The eigenvalues $E_{\pm}(\tau)$ and eigenvectors $|u_{0\pm}(\tau)\rangle$ of the instantaneous $\hat{H}(\tau)$, which constitute the adiabatic basis, are

$$E_{\pm}(\tau) = \pm H(\tau) = \pm\sqrt{(X^2+Z^2)} \tag{5}$$

and

$$|u_{0+}(\tau)\rangle = \begin{pmatrix}\cos\frac{1}{2}\theta\\ \sin\frac{1}{2}\theta\end{pmatrix}, \quad |u_{0-}(\tau)\rangle = \begin{pmatrix}\sin\frac{1}{2}\theta\\ -\cos\frac{1}{2}\theta\end{pmatrix}. \tag{6}$$

We assume $H > 0$ for all real τ, that is no degeneracies of the adiabatic states. (5) and (6) are the ingredients of the lowest-order small-ϵ solutions of (3):

$$|\psi_{\pm}(\tau)\rangle \approx |\psi_{0\pm}(\tau)\rangle \equiv \exp\left\{\mp\frac{\mathrm{i}}{\epsilon}\int_0^{\tau}\mathrm{d}\tau' H(\tau')\right\}|u_{0\pm}(\tau)\rangle. \tag{7}$$

$|\psi_{0+}\rangle$ starts, and remains, in the upper eigenstate of the instantaneous $\hat{H}(\tau)$, and $|\psi_{0-}\rangle$ starts and remains in the lower: there are no transitions in this approximation.

In the next section we construct superadiabatic approximations $|\psi_{n\pm}(\tau)\rangle$, representing $|\psi\rangle$ to successively higher orders in ϵ. None of these bases describe transitions because transitions are of infinite order $(\exp(-1/\epsilon))$ in ϵ. But we can of course use $|\psi_{n+}(\tau)\rangle$ and $|\psi_{n-}(\tau)\rangle$ as basis states in an exact representation of $|\psi\rangle$, namely

$$\begin{aligned}|\psi(\tau)\rangle &= c_{n+}(\tau)\,|\psi_{n+}(\tau)\rangle + c_{n-}(\tau)\,|\psi_{n-}(\tau)\rangle\\ &\equiv \hat{U}_n(\tau)\,|c_n(\tau)\rangle.\end{aligned} \tag{8}$$

Here $|c\rangle$ is the column vector with components c_+ and c_-, and $\hat{U}_n$ the time-dependent unitary operator

$$\hat{U}_n(\tau) \equiv \begin{pmatrix}\psi_{n+,1} & \psi_{n-,1}\\ \psi_{n+,2} & \psi_{n-,2}\end{pmatrix}. \tag{9}$$

Transforming (3) to the nth superadiabatic basis, we find that the coefficients $|c_n\rangle$ obey the Schrödinger equation

$$\mathrm{i}\epsilon|\dot{c}_n\rangle = \hat{H}_n|c_n\rangle, \quad \text{where} \quad \hat{H}_n = \hat{U}_n^{+}(\hat{H} - \mathrm{i}\epsilon\mathrm{d}_{\tau})\,\hat{U}_n. \tag{10}$$

An elementary calculation gives the explicit form

$$\hat{H}_n = \begin{pmatrix}H_{n++} & H_{n+-}\\ H_{n-+} & H_{n--}\end{pmatrix}, \tag{11}$$

where

$$H_{n\alpha\beta} = \langle\psi_{n\alpha}|\,\hat{H} - \mathrm{i}\epsilon\mathrm{d}_{\tau}|\psi_{n\beta}\rangle, \quad (\alpha,\beta) = (+,-). \tag{12}$$

Thus the more accurately $|\psi_{n\pm}\rangle$ approximate the solutions $|\psi\rangle$ of (3), the smaller are the elements of $\hat{H}_n$ and the smaller are the variations in $|c_n\rangle$. We shall find (§4) that the superadiabatic sequence $\hat{H}_n$ is asymptotic, that is the $\hat{H}_n$ get rapidly smaller at first but ultimately diverge. Our universal transition history will result (§5) from stopping at the n for which $\hat{H}_n$ is smallest.

Transitions between $|\psi_{n+}\rangle$ and $|\psi_{n-}\rangle$ are induced by the off-diagonal elements of $\hat{H}_n$. These can be calculated by lowest-order perturbation theory applied to (10). We consider (without losing any essential generality) the initial $|\psi\rangle$ which starts in the upper eigenstate, i.e.

$$|c_n(-\infty)\rangle = \begin{pmatrix}1\\0\end{pmatrix} \tag{13}$$

apart from a phase factor, irrelevant here. Then the transition amplitude $c_{n-}(\tau)$ can be calculated on the assumption that $c_{n+}(\tau)$ remains unity. The result is

$$c_{n-}(\tau) \approx -\frac{\mathrm{i}}{\epsilon}\exp\left\{-\frac{\mathrm{i}}{\epsilon}\int_0^\tau \mathrm{d}\tau'\, H_{n--}(\tau')\right\} \times \int_{-\infty}^{\tau} \mathrm{d}\tau'\, H_{n-+}(\tau')\exp\left\{+\frac{\mathrm{i}}{\epsilon}\int_0^{\tau'} \mathrm{d}\tau''\, H_{n--}(\tau'')\right\}. \tag{14}$$

It is not obvious that this perturbation procedure is valid. Indeed it is well known (Davis & Pechukas 1976) that in the usual adiabatic basis $n = 0$ it gives the wrong final amplitude $c_{0-}(+\infty)$. But we shall show in §6 that it is valid for high-order superadiabatic bases, i.e. large n.

3. Construction of superadiabatic bases

Write the exact solutions $|\psi_+\rangle$ and $|\psi_-\rangle$ of (3) as formal power series in ϵ whose lowest terms are the adiabatic approximations (7):

$$|\psi_\pm(\tau)\rangle = \exp\left\{\mp\frac{\mathrm{i}}{\epsilon}\int_0^\tau \mathrm{d}\tau'\, H(\tau')\right\} \sum_{m=0}^{\infty} \epsilon^m |u_{m\pm}(\tau)\rangle. \tag{15}$$

The sequence of superadiabatic bases then consists of the truncated sums

$$|\psi_{n\pm}(\tau)\rangle = \exp\left\{\mp\frac{\mathrm{i}}{\epsilon}\int_0^\tau \mathrm{d}\tau'\, H(\tau')\right\} \sum_{m=0}^{n} \epsilon^m |u_{m\pm}(\tau)\rangle. \tag{16}$$

Here it will be necessary only to find the solution $|\psi_+\rangle$. We realize that $|u_{0+}\rangle$ and $|u_{0-}\rangle$ (equations (6)) form a complete set, and expand

$$|u_{m+}(\tau)\rangle = a_m(\tau)\,|u_{0+}(\tau)\rangle + b_m(\tau)\,|u_{0-}(\tau)\rangle; \tag{17}$$

a_m and b_m will be determined by substitution into (3) and the conditions

$$a_0(\tau) = 1, \quad b_0(\tau) = 0, \quad a_m(-\infty) = b_m(-\infty) = 0\ (m > 0). \tag{18}$$

The calculation makes use of the fact that $|\dot{u}_{0\pm}\rangle$ are orthogonal to $|u_{0\pm}\rangle$: from (6),

$$|\dot{u}_{0\pm}\rangle = \mp\tfrac{1}{2}\dot{\theta}|u_{0\mp}\rangle. \tag{19}$$

Elementary calculations then give

$$b_m = -2\dot{a}_m/\dot{\theta} \tag{20}$$

and the recurrence relation

$$\dot{a}_m = -(\mathrm{i}/2H)\left(\tfrac{1}{4}\dot{\theta}^2 a_{m-1} + \ddot{a}_{m-1} - (\ddot{\theta}/\dot{\theta})\,\dot{a}_{m-1}\right) \tag{21}$$

To calculate the matrix elements (12) in the transition amplitude integral (14), we need to know the effect of operating with $\hat{H} - \mathrm{i}\epsilon\,\mathrm{d}_\tau$ on $|\psi_{n+}\rangle$. This has to be of order ϵ^{n+1}, and direct substitution of (16) and use of (20) and (21) give

$$(\hat{H} - \mathrm{i}\epsilon\,\mathrm{d}_\tau)\,|\psi_{n+}\rangle = -\epsilon^{n+1}\frac{4H\dot{a}_{n+1}}{\dot{\theta}}\exp\left\{-\frac{\mathrm{i}}{\epsilon}\int_0^\tau \mathrm{d}\tau'\,H(\tau')\right\}|u_{0-}\rangle. \tag{22}$$

Thus, to lowest order in ϵ,

$$H_{n-+} \approx -\epsilon^{n+1}\frac{4H\dot{a}_{n+1}}{\dot{\theta}}\exp\left\{-\frac{2\mathrm{i}}{\epsilon}\int_0^\tau \mathrm{d}\tau'\,H(\tau')\right\}. \tag{23}$$

A similar argument shows that H_{n--} is of order ϵ^{n+2} (actually H_{0--} vanishes identically).

To evaluate (14) to lowest order in ϵ, that is in the adiabatic limit, we can replace the exponentials by unity (since the exponents are of order ϵ^{n+1}), and obtain the nth superadiabatic transition amplitude as

$$c_{n-}(\tau) \approx 4\mathrm{i}\epsilon^n \int_{-\infty}^{\tau} \mathrm{d}\tau'\,\frac{H\dot{a}_{n+1}}{\dot{\theta}}\exp\left\{-\frac{2\mathrm{i}}{\epsilon}\int_0^{\tau'} \mathrm{d}\tau''\,H(\tau'')\right\}. \tag{24}$$

At this point it is natural to define the new variable (proportional to action)

$$w(\tau) \equiv 2\int_0^\tau \mathrm{d}\tau'\,H(\tau'), \tag{25}$$

which will play an important part in what follows. In terms of w,

$$c_{n-}(\tau) \approx 2\mathrm{i}\epsilon^n \int_{-\infty}^{w(\tau)} \mathrm{d}w\,\frac{a'_{n+1}}{\theta'}\exp\left\{-\frac{\mathrm{i}w}{\epsilon}\right\}, \tag{26}$$

where here and hereafter primes denote w derivatives.

4. High-order superadiabatic asymptotics

Direct iteration of (21), starting from $a_0 = 1$ and $\dot{\theta}(\tau)$ as defined by the hamiltonian (4), generates a sequence a_m of increasingly complicated functionals of $\dot{\theta}$ and hence increasingly complicated functions of τ. And of course the functions a_m depend on the details of the time dependence of $\hat{H}$. Yet it is a remarkable fact that as $m \to \infty$ (the 'asymptotics of the asymptotics') the a_m become both simple and universal in form.

To see how this happens, consider first the zero-order (ordinary adiabatic) basis $n = 0$, and the problem of evaluating the final amplitude $c_-(+\infty)$. From the first iteration of (21), (26) gives

$$c_{0-}(\infty) \approx \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}w\,\theta'\exp\left\{-\frac{\mathrm{i}w}{\epsilon}\right\}. \tag{27}$$

The integrand is analytic near the real axis, so we can displace the contour down into the lower half-plane until it hits the first singularity w_c of θ' (regarded as a function of w). For small ϵ this singularity (with the smallest value of $-\operatorname{Im} w_c$) gives the dominant contribution to $c_0(+\infty)$. The contribution depends on the residue of θ' at w_c.

What is the origin of the singularities of θ'? One possibility is that the elements $X(\tau), Z(\tau)$ of $\hat{H}$ themselves have singularities. We ignore this possibility, although it is interesting (Fishman *et al.* 1989), and concentrate on the more common situation where the singularities come from complex adiabatic degeneracies, that is complex simple zeros of the eigenvalues $H(\tau)$. It was discovered by Davis & Pechukas (1977) (see also Berry & Mount 1972) in an argument which for the sake of completeness is repeated in Appendix B, that at such a zero θ' has a simple pole with residue $+\frac{1}{3}\mathrm{i}$, that is

$$\theta' \approx +\mathrm{i}/3(w-w_c) \quad \text{for } w \text{ near } w_c. \tag{28}$$

Contour integration now gives

$$c_{0-}(+\infty) \approx \tfrac{1}{3}\pi \exp\{-\mathrm{i}w_c/\epsilon\} \tag{29}$$

to which we will return in §6.

This is indeed universality, because the form of the result is independent of all details of $\hat{H}$. The universality stems from that of the function θ' near w_c. But this is not the problem we wanted to solve. For the transition history (rather than the final amplitude) we need to be on the real τ (or w) axis, rather than in the complex plane, and we seek the amplitudes for large superadiabatic order n, rather than $n = 0$.

Note, however, that because of the derivatives in (21) (or its equivalent in the w variable) the effect of high iterations is to magnify the singularity at w_c. Thus the domain surrounding w_c, in which the singularity will dominate a_m, will get larger as m increases. Eventually the domain of influence will reach the real axis, so that high-order a_ms are given by the exact solution of (21) with the local form (28) substituted for θ'. This is Darboux's 'principle of the nearest singularity', clearly explained, and applied to the determination of late terms of a variety of asymptotic series, by Dingle (1973). Thus does the universality near w_c propagate to universality on the real axis. (Of course, on the real axis a_m will also be influenced by the conjugate singularity w_c^* in the upper half-plane, but for large m the contributions from w_c and w_c^* simply add.)

To carry out this programme, we must solve (21) with (28). After transforming from τ to w, we find

$$a'_m = \mathrm{i}\left(\frac{a_{m-1}}{36(w-w_c)^2} - \frac{a'_{m-1}}{w-w_c} - a''_{m-1}\right). \tag{30}$$

This has the exact solution

$$a_m = \frac{\mathrm{i}^m (m-\frac{7}{6})!\,(m-\frac{5}{6})!}{(w-w_c)^m\, m!\,(-\frac{7}{6})!\,(-\frac{5}{6})!}. \tag{31}$$

The quantity appearing in (26) is thus

$$2\mathrm{i}\frac{a'_{n+1}}{\theta'} = \frac{\mathrm{i}^{n+1}(n-\frac{1}{6})!\,(n-\frac{5}{6})!\,(1+1/(6n))}{(w-w_\mathrm{c})^{n+1}\,(n-1)!\,(-\frac{1}{6})!\,(-\frac{5}{6})!}. \tag{32}$$

Because of Stirling's formula the factorials simplify, and after adding the contribution from w_c^* (for which the analogue of (28) has a minus sign) we obtain, on the real axis,

$$2\mathrm{i}\frac{a'_{n+1}}{\theta'} \approx \frac{n!\,\mathrm{i}^{n+1}}{2\pi}\left(\frac{1}{(w-w_\mathrm{c})^{n+1}} - \frac{1}{(w-w_\mathrm{c}^*)^{n+1}}\right). \tag{33}$$

Note that because of the $n!$ the formal series for (15) for $|\psi_+\rangle$ always diverges. This must happen. If it did not, then, since all approximants $|\psi_{+n}\rangle$ are asymptotic to the same adiabatic eigenstate at $\tau = -\infty$ and $\tau = +\infty$, there would be no transition.

5. Universal transition history

Without loss of generality it is possible to take w_c as purely imaginary, i.e.

$$w_\mathrm{c} = -\mathrm{i}|w_\mathrm{c}|. \tag{34}$$

This amounts to choosing the origin of τ at the point where the locus

$$\mathrm{Re}\int_{\tau}^{\tau_\mathrm{c}} \mathrm{d}\tau'\,H(\tau') = 0$$

(a Stokes line emanating from w_c) crosses the real τ axis.

From now on we consider w real. It will emerge that the transition occurs in a range of $w \ll |w_\mathrm{c}|$, so we expand (33) in $w/|w_\mathrm{c}|$ and for $n \gg 1$:

$$2\mathrm{i}\frac{a'_{n+1}}{\theta'} \approx \frac{n^{n+\frac{1}{2}}\exp(-n)}{\sqrt{(2\pi)}\,|w_\mathrm{c}|^{n+1}}\exp\left\{-\frac{(n+1)\,w^2}{2|w_\mathrm{c}|^2}\right\} \times\left[\exp\left\{\mathrm{i}\frac{(n+1)\,w}{|w_\mathrm{c}|}\right\} + (-1)^n\exp\left\{-\mathrm{i}\frac{(n+1)\,w}{|w_\mathrm{c}|}\right\}\right]. \tag{35}$$

Note that the first complex exponential (from the lower half-plane) reduces the oscillations of the integrand in (26), whereas the contribution from the upper half-plane gives a faster oscillation and hence, because of the analytic integrand, a much smaller contribution which can therefore be neglected.

Note further that by choosing

$$n = n_\mathrm{c} \equiv \mathrm{Int}\,|w_\mathrm{c}/\epsilon| \tag{36}$$

the oscillations in (26) can be eliminated altogether, so that

$$2\mathrm{i}\epsilon^n\frac{a'_{n+1}}{\theta'}\exp\left\{-\mathrm{i}\frac{w}{\epsilon}\right\} \approx \frac{1}{(2\pi|w_\mathrm{c}|)^{\frac{1}{2}}}\exp\left\{-\frac{w^2}{2\epsilon|w_\mathrm{c}|}\right\}\exp\left\{-\frac{|w_\mathrm{c}|}{\epsilon}\right\}. \tag{37}$$

More careful analysis (carried out for similar problems by Berry (1989*a*, 1990*a*)) shows that the elimination is insensitive to deviations $|n-n_c|$ of order unity. Substituting into (26), we find the following remarkably simple result:

$$c_{n_c^-}(\tau) \approx \tfrac{1}{2}[1+\mathrm{Erf}\{\sigma\}]\exp\{-|w_c|/\epsilon\}, \tag{38}$$

where Erf is the error function (Abramowitz & Stegun 1964) and

$$\sigma \equiv \frac{w(\tau)}{\surd(2\epsilon|w_c|)} = H(0)\,t \sqrt{\left[\delta/\hbar \left| \int_0^{\tau_c} \mathrm{d}\tau\, H(\tau)\right|\right]}. \tag{39}$$

(Here the integral for $w(\tau)$ has been linearized, a procedure easily justified by the arguments surrounding (40)–(42) below.)

Equation (38) is the universal transition history. It depends only on the properties of the level separation along the Stokes line from the complex degeneracy τ_c to the real axis. The amplitude rises monotonically to its exponentially small final value. This smooth rise is a consequence of optimal superadiabaticity. For $n \ll n_c$ the exponentially small final amplitude emerges from much larger oscillations, of order ϵ^{n+1}, spread over a large interval of the τ axis. For $n \gg n_c$ the oscillations are again large because of the factorial divergence in the asymptotic coefficients (33) and (35). Note that n_c is precisely the order of superadiabaticity that optimizes the asymptotic approximant (16) for $|\psi_+\rangle$.

Our optimal history furnishes a natural measure of the time t_{trans} during which the qauntum transition takes place. This is the time for σ to increase from -1 to $+1$. From (39), we obtain

$$t_{\mathrm{trans}} = 2\sqrt{\left[\hbar \left| \int_0^{\tau_c} \mathrm{d}\tau\, H(\tau)\right| \Big/ \delta H^2(0)\right]}. \tag{40}$$

In the familiar Landau–Zener model, with $X = \text{const.} \equiv \varDelta$ and $Z = \tau$, we have

$$H(\tau) = (\varDelta^2+\tau^2)^{\frac{1}{2}} \tag{41}$$

so that $\tau_c = -\mathrm{i}\varDelta$ and

$$t_{\mathrm{trans}} = \surd(\pi\hbar/\delta). \tag{42}$$

By contrast, the transition in the ordinary adiabatic representation takes the much longer time $\varDelta/\delta$ (Mullen *et al.* 1989).

6. Solution of the $\frac{1}{3}\pi$ problem

In the nth superadiabatic basis, the final amplitude is obtained by deforming the contour in (26) around the pole in (32). The result is

$$c_n(+\infty) \approx A_n \exp\{-\mathrm{i}w_c/\epsilon\} = A_n \exp\{-|w_c|/\epsilon\}, \tag{43}$$

where

$$A_n = \frac{2\pi(n+\frac{1}{6})!\,(n-\frac{1}{6})!}{(-\frac{1}{6})!\,(-\frac{5}{6})!\,(n!)^2}. \tag{44}$$

In the usual adiabatic basis, $n = 0$ and $A_0 = \frac{1}{3}\pi$, as we found before (equation (29)). This result is wrong: the exact adiabatic coefficient is 1, not $\frac{1}{3}\pi$. The error is an artefact of perturbation theory, all orders of which (in the $n = 0$ basis) give exponentially small contributions to the amplitude. As n increases, however, A_n renormalizes to unity, indicating that lowest-order perturbation theory becomes better until, for $n \gg 1$ (as with optimal superadiabaticity) it gives the correct adiabatic amplitude (see Berry (1990*a*) for a discussion of the reason for the improvement).

The first few A_n are

$$A_0 = \tfrac{1}{3}\pi = 1.047, \quad A_1 = \tfrac{35}{36}A_0 = 1.018, \quad A_2 = \tfrac{143}{144}A_1 = 1.011. \tag{45}$$

In the limit, we have

$$A_n = 1 + 1/36n + \dots \quad (n \gg 1). \tag{46}$$

7. Possible experiments

Equations (3) and (4) describe the evolution of the state of a spin-$\frac{1}{2}$ quantum particle with a magnetic moment (e.g. a neutron) coupled to a time-dependent magnetic field $\boldsymbol{H}(\tau)$ with components $X(\tau), Z(\tau)$. At any time τ, the state of the system can be probed by measuring the component of the spin operator $\hat{\boldsymbol{S}}$ in some direction with unit vector $\boldsymbol{e}$, that is

$$\langle \psi | \hat{\boldsymbol{S}} \cdot \boldsymbol{e} | \psi \rangle, \tag{47}$$

where

$$\hat{\boldsymbol{S}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{48}$$

We seek experiments to measure the nth superadiabatic transition probability $|c_{n-}(\tau)|^2$. An elementary exercise in quantum mechanics shows that the required direction is

$$\boldsymbol{e}_n = \langle \psi_{n+} | \hat{\boldsymbol{S}} | \psi_{n+} \rangle \tag{49}$$

for then

$$\langle \psi | \hat{\boldsymbol{S}} \cdot \boldsymbol{e} | \psi \rangle = |c_{n+}(\tau)|^2 - |c_{n-}(\tau)|^2 = 1 - 2|c_{n-}(\tau)|^2. \tag{50}$$

The lowest-order (usual adiabatic) observable is the spin in the direction

$$\epsilon_0 = \boldsymbol{H}/H \equiv \boldsymbol{h} \tag{51}$$

of the instantaneous field. The higher-order directions $\boldsymbol{e}_n$ could be obtained by substituting the truncated power series (16) into (49). A more direct procedure, which to lowest order in ϵ gives the same result, is to truncate the formal adiabatic series for the moving spin expectation

$$\boldsymbol{S} = \langle \psi | \hat{\boldsymbol{S}} | \psi \rangle. \tag{52}$$

In terms of the variable w, $\boldsymbol{S}$ satisfies the equation

$$\boldsymbol{S}' = (1/\epsilon)\, \boldsymbol{h} \wedge \boldsymbol{S}, \tag{53}$$

where of course both $\boldsymbol{h}$ and $\boldsymbol{S}$ are functions of w. The desired higher-order measuring directions are the truncations

$$\boldsymbol{e}_n \equiv \sum_{m=0}^{n} \epsilon^m \boldsymbol{S}_m \tag{54}$$

of the formal series

$$\boldsymbol{S} = \sum_{m=0}^{\infty} \epsilon^m \boldsymbol{S}_m, \quad \boldsymbol{S}_0 = \boldsymbol{h}. \tag{55}$$

Substitution into (53) gives the implicit recurrence relation

$$\boldsymbol{h} \wedge \boldsymbol{S}_{m+1} = \boldsymbol{S}'_m, \tag{56}$$

whose inversion gives (after a little algebra) the explicit inversion

$$\boldsymbol{S}_{m+1} = \boldsymbol{S}'_m \wedge \boldsymbol{h} + \boldsymbol{h} \int_{-\infty}^{w} \mathrm{d}w\, \boldsymbol{S}'_m \cdot (\boldsymbol{h} \wedge \boldsymbol{h}'). \tag{57}$$

In this way it is possible, in principle, to follow any of the superadiabatic transition histories $|c_{n-}(\tau)|^2$, including that for the optimal order $n = n_c$. Of course such experiments would be difficult, because the different measurement direction histories $\boldsymbol{e}_n(\tau)$ differ only slightly (by successively higher powers of ϵ). This explicit description of the exquisite sensitivity of the measured quantity to the chosen observable is one of the main outcomes of this work.

8. Concluding remarks

I have shown that among bases close to the adiabatic eigenstates and coinciding with them at $t = \pm\infty$, there is an optimal basis, in which the exponentially weak transition occurs smoothly and without oscillations. In this superadiabatic basis, the transition occurs in a universal and measurable manner over a time of order $(\hbar/\delta)^{\frac{1}{2}}$ where δ is the adiabatic parameter. The mechanism of universality is a kind of reverse analytic continuation, induced by the sequence of superadiabatic transformations, from the complex degeneracy back to the real axis.

It is desirable to have rigorous mathematical justification for some of the steps in the argument, for example the spreading of the singularity to include the real axis, and the superposition of contributions from the two conjugate complex degeneracies.

Most useful would be a proof (or disproof) of the optimality of the error-function transition history. In what sense is it the most rapid possible transition? This is a subtle question, for it is easy to construct bases in which the transition has any desired history. An example is the basis that follows the exact $|\psi\rangle$ until long after the direction of $\boldsymbol{H}$ has ceased to change, and then switches abruptly to the original adiabatic state; in this basis the transition too is abrupt. But finding this basis requires the exact solution of Schrödinger's equation. The question should be restricted to explicitly analytically constructable bases, such as the sequence used here.

Various extensions can be envisaged for which the optimal superadiabatic transition history might be different from the universal one. For example, several complex degeneracies could have equal values of $\operatorname{Im} w_c$ and so contribute interfering exponentials of the same magnitude. Or, $\hat{H}$ could itself have complex singularities with $\operatorname{Im} w_c$ smaller than its degeneracy value, as in the example studied by Fishman *et al.* (1989). Or, more than two states could be involved in the transition in an essential way, as discussed by Hwang & Pechukas (1977).

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Appendix A

This is the proof that any 2×2 hermitian matrix can be transformed into the form (4). The most general case is

$$\hat{H}(\tau) = \begin{pmatrix} Z(\tau)+A(\tau) & X(\tau)\exp\{-\mathrm{i}\phi(\tau)\} \\ X(\tau)\exp\{\mathrm{i}\phi(\tau)\} & -Z(\tau)+A(\tau) \end{pmatrix}. \tag{A 1}$$

Write the solution of (3) as

$$|\psi(\tau) = \hat{U}(\tau)|\psi'(\tau), \tag{A 2}$$

where

$$\hat{U}(\tau) = \exp\left\{-\frac{\mathrm{i}}{\epsilon}\int_0^\tau \mathrm{d}\tau' A(\tau')\right\}\begin{pmatrix} \exp\{-\frac{1}{2}\mathrm{i}\phi(\tau)\} & 0 \\ 0 & \exp\{\frac{1}{2}\mathrm{i}\phi(\tau)\} \end{pmatrix}. \tag{A 3}$$

Then $|\psi'\rangle$ obeys a Schrödinger equation with hamiltonian which indeed has the form (4):

$$\hat{H}' = \hat{U}^{+}(\hat{H}-\mathrm{i}\epsilon d_\tau)\,\hat{U} = \begin{pmatrix} Z'(\tau) & X'(\tau) \\ X'(\tau) & -Z'(\tau) \end{pmatrix}, \tag{A 4}$$

where

$$X'(\tau) = X(\tau), \quad Z'(\tau) = Z(\tau) - \tfrac{1}{2}\mathrm{i}\epsilon\dot{\phi}(\tau). \tag{A 5}$$

Appendix B

This is the derivation of (28), following Davis & Pechukas (1976). Let τ_c be a complex simple zero of $H = (X^2+Z^2)^{\frac{1}{2}}$. Near τ_c, X and Z, being analytic, can be written in the form

$$X = \alpha + \beta(\tau-\tau_c), \quad Z = \pm\mathrm{i}\alpha + \gamma(\tau-\tau_c). \tag{B 1}$$

Thus

$$H^2 \approx 2\alpha(\tau-\tau_c)\,(\beta\pm\mathrm{i}\gamma) \quad \text{near } \tau_c. \tag{B 2}$$

We now find

$$\dot{\theta} = \cos^2\theta(\tan\theta)^{\cdot} = \frac{Z^2}{H^2}\left(\frac{X}{Z}\right)^{\cdot} = \frac{\dot{X}Z-\dot{Z}X}{H^2}$$

$$\approx \frac{\pm\mathrm{i}\beta\alpha-\alpha\gamma}{2\alpha(\tau-\tau_c)\,(\beta\pm\mathrm{i}\gamma)} = \frac{\pm\mathrm{i}}{2(\tau-\tau_c)}. \tag{B 3}$$

Because H has a square-root branch-point at τ_c, w (equation (25)) has the form

$$w = w_c + \tfrac{4}{3}(\tau-\tau_c)^{\frac{3}{2}}[2\alpha(\beta\pm\mathrm{i}\gamma)]^{\frac{1}{2}}. \tag{B 4}$$

Direct substitution in (C 3) gives

$$\theta' = \pm \mathrm{i}/3(w-w_c), \tag{B 5}$$

which is (28) apart from a sign ambiguity.

Because θ' is real for all real τ, the signs in (B 5) must be opposite for the poles at w_c and w_c^*. The absolute sign at w_c (in the lower half-plane) is a matter of convention. With any given convention, the sign reverses if ϵ reverses, that is if the hamiltonian history is reversed. There is therefore no loss of essential generality in choosing $+$, as in (28).

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