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Universal transition prefactors derived by superadiabatic renormalization

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Abstract. For time-dependent two-state quantum systems, the transition probability is exponentially small in the adiabatic parameter ε, with the exponent determined by a transition point t_c in the complex time plane. Here we study the ε-independent prefactors associated with different sorts of transition point (which need not correspond to complex degeneracies of the adiabatic energy). Unlike previous approaches the method we use does not make use of special functions. It consists of applying first-order perturbation theory to the Schrödinger equation obtained by transforming to a series of 'superadiabatic' bases clinging ever more closely to the evolving state. If the original matrix elements share a leading singularity $(t-t_c)^r$, and their fractional deviation from this is $(t-t_c)^s$, the prefactor is

$$4\sin^2\left\{\frac{\pi s}{2(2r+s+2)}\right\}.$$

This is universal in the sense of being invariant under time reparametrization and quantum changes of frame.

1. Introduction

In the simplest model for quantum transitions, a system with two states evolves under a time-dependent Hamiltonian operator $H(t)$. This has many physical applications (see e.g. Garraway *et al* 1993). It is well known (see e.g. Davis and Pechukas 1976) that for Hamiltonians which are analytic on the real time axis the probability for a transition after infinite time from one of the instantaneous eigenstates to the other is exponentially small in the adiabatic parameter ε describing the speed with which $H(t)$ varies. The exponent involves

$$w_c = 2\int_0^{t_c} \mathrm{d}t\, E(t) \tag{1}$$

where $E(t)$ is the instantaneous energy, defined as the eigenvalue of $H(t)$ which is positive for real t (we assume $E(t)$ has no real zeros), and t_c is a point in the complex plane where the adiabatic transition can be considered to originate. Therefore these transitions describe real physics in the complex plane. In the most familiar case, the transition point t_c is a simple zero of $E^2(t)$, and (when $H(t)$ is real symmetric) the ε-independent prefactor multiplying the exponential is unity.

Here we are concerned with the different prefactors that can occur when the transition point is not a simple zero of $E^2(t)$. Demkov *et al* (1978) calculated a class of such

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prefactors, in which t_c is a higher-order zero, and Joye (1993) has provided a rigorous treatment that also covers more general sorts of transition point. Earlier, Pokrovskii and Khalatnikov (1961) found the prefactors for the analogous problem of above-barrier reflection in the semiclassical approximation. All these authors use a comparison-equation technique, in which $H(t)$ is approximated near t_c and the resulting approximate Schrödinger equation solved exactly in terms of hypergeometric functions.

We have two reasons for presenting another calculation of these prefactors: first, to emphasize their wide universality class and, second, because of the independent interest of the method we use. This is first-order perturbation theory, applied not to states in the usual adiabatic basis (which is known to give the wrong prefactor) but to a sequence of 'superadiabatic' bases that cling ever more closely to the evolving state; the corresponding sequence of prefactors renormalises onto the correct value. No knowledge of special functions is required in this method, which can therefore be regarded as elementary. It was introduced by Berry (1990a) and applied to obtain the prefactor of unity for simple transition points, in a paper whose main purpose was to study the history of the transition, that is the growth of the probability amplitude from zero to its exponentially small final value (see also Berry 1990b and Lim and Berry 1991).

Confusion should be avoided between the prefactors we study here and the recently-discovered 'geometric amplitudes' (Berry 1990c, Joye *et al* 1991, Zwanziger *et al* 1991). Geometric amplitudes are also independent of ε, but arise from spinor rotations associated with the complex Hermitian nature of $H(t)$, rather than from more complicated transition points.

2. Preliminaries

We seek approximate solutions of the Schrödinger equation

$$i\varepsilon\dot{\Psi}(t)=H(t)\Psi(t) \tag{2}$$

in the adiabatic limit of small ε. Here the dot denotes differentiation with respect to time, and

$$\begin{aligned}\Psi(t)&\equiv\begin{pmatrix}\Psi_1(t)\\ \Psi_2(t)\end{pmatrix}\\ H(t)&\equiv\begin{pmatrix}Z(t) & X(t)\\ X(t) & -Z(t)\end{pmatrix}\equiv E(t)\begin{pmatrix}\cos\theta(t) & \sin\theta(t)\\ \sin\theta(t) & -\cos\theta(t)\end{pmatrix}.\end{aligned} \tag{3}$$

We assume that $\theta(t)$ is asymptotically constant as $t\to\pm\infty$. The adiabatic states (proportional to instantaneous eigenstates of $H(t)$) are

$$\psi_\pm(t)=\exp\left\{\mp\frac{i}{\varepsilon}\int_0^t dt'\,E(t')\right\}u_\pm(t)$$

where (4)

$$u_+(t)\equiv\begin{pmatrix}\cos\frac{1}{2}\theta(t)\\ \sin\frac{1}{2}\theta(t)\end{pmatrix}\qquad u_-(t)\equiv\begin{pmatrix}-\sin\frac{1}{2}\theta(t)\\ \cos\frac{1}{2}\theta(t)\end{pmatrix}$$

Using these as a basis, we write the exact solutions of (2) as

$$\Psi(t)=c_+(t)\psi_+(t)+c_-(t)\Psi_-(t). \tag{5}$$

As initial state we choose

$$c_+(-\infty)=1 \qquad c_-(-\infty)=0 \tag{6}$$

so that the desired transition probability is

$$P=|c_-(+\infty)|^2. \tag{7}$$

It is easy to see that the conventional view, in which adiabatic transitions originate in complex zeros of $E(t)$, misses the essence of the problem. For all zeros can be eliminated by the transformation

$$t\to w \qquad \text{where} \qquad w(t)\equiv 2\int_0^t \mathrm{d}t'\,E(t') \tag{8}$$

because this converts (2) into

$$\mathrm{i}\varepsilon\begin{pmatrix}\Psi_1'\\ \Psi_2'\end{pmatrix}=\tfrac{1}{2}\begin{pmatrix}\cos\theta & \sin\theta\\ \sin\theta & -\cos\theta\end{pmatrix}\begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix} \tag{9}$$

(where primes denote differentiation with respect to w), in which the instantaneous energy is constant. (The transformation $t\to w$ is not invertible at zeros of $E(t)$, but the branch can be determined by analytic continuation from the real axis.) We will obtain a formula for P which is invariant under all time reparameterizations, not just the choice (8). Two particular Hamiltonians for which E is constant, and whose prefactors we will study in section 5, are H_A and H_B, defined by

$$\begin{aligned} X_A(t)&=\frac{1}{\sqrt{1+t^2}} & Z_A(t)&=\frac{t}{\sqrt{1+t^2}}\\ X_B(t)&=\operatorname{sech}(\tfrac{1}{2}\pi t) & Z_B(t)&=\tanh(\tfrac{1}{2}\pi t). \end{aligned} \tag{10}$$

H_A was also studied by Suominen *et al* (1991); H_B was introduced by Demkov and Kunike (1969) (see also Suominen and Garraway 1992).

The true origin of adiabatic transitions is revealed by the further transformation to the adiabatic basis (5). The evolution law for the amplitudes $c_\pm$ (now regarded as functions of w) is

$$c_\pm'(w)=\pm\tfrac{1}{2}\theta'(w)\exp\left\{\pm\mathrm{i}\frac{w}{\varepsilon}\right\}c_\mp(w). \tag{11}$$

What causes adiabatic transitions are therefore the (complex) singularities of $\theta'(w)$, and these will play a central role in what follows. In section 4 we shall find that for a very wide class of functions $X(t)$ and $Z(t)$ the singularities at $w=w_c$ (cf (1)) are simple poles, that is

$$\theta'(w)\to-\frac{\mathrm{i}\gamma}{w-w_c} \tag{12}$$

where γ is a real constant with the universality property that it depends only on the type of singularity and not on any associated coefficients. This universality and its

significance were first appreciated by Davis and Pechukas (1976) for the particular case of a simple zero of $E^2(t)$, where they found $\gamma = 1/3$.

From (7) and (11), the transition probability is

$$P = \left| -\tfrac{1}{2} \int_{-\infty}^{\infty} dw\, c_+(w)\theta'(w) \exp\left\{ -i\frac{w}{\varepsilon} \right\} \right|^2 \tag{13}$$

In a first approximation to P, we use lowest-order perturbation theory, in which it is assumed that $c_+(t)$ preserves its initial value of unity. Then (13) depends on the singularities of $\theta'(w)$ in the lower half-plane. Assuming that there is one closest to the real axis (that is, ignoring the 'Stückelberg oscillations' arising from the interference of singularities with equal Im w), we use (12) to obtain

$$P \approx P_0 = \pi^2\gamma^2 \exp\left\{ -2\frac{|\mathrm{Im}\, w_c|}{\varepsilon} \right\} \tag{14}$$

As is well known, in this lowest-order perturbation result the prefactor $\pi^2\gamma^2$ is wrong. One way to get the right result is to iterate the equations (11) to obtain the full perturbation series for c_-. This was done by Davis and Pechukas (1976) for a simple zero, and by Berry (1982) for above-barrier reflection from a turning point of arbitrary order. For small ε all terms involve the same exponential but different (ε-independent) multipliers, whose sum is the correct adiabatic prefactor. In what follows, we employ a different procedure.

3. Superadiabatic renormalization

As explained by Berry (1990a)—to which we refer for many details of the argument of this section—first-order perturbation theory fails because the quantity being calculated is exponentially small and therefore beyond all orders in the small parameter ε. However, first-order perturbation theory can be used if the representation (5), in terms of the adiabatic basis (4) is replaced by the nth-order superadiabatic representation

$$\Psi(w) = c_{n+}(w)\psi_{n+}(w) + c_{n-}(t)\Psi_{n-}(w) \tag{15}$$

for sufficiently large n. Here $\psi_{n\pm}$ are the series solutions of (2) in powers of ε, truncated at ε^n, namely

$$\psi_{n\pm}(w) = \exp\left\{ \mp\frac{iw}{2\varepsilon} \right\} \sum_{m=0}^{n} \varepsilon^m u_{m,\pm}(w) \tag{16}$$

where the vectors $u_{m,\pm}(w)$ will shortly be determined. The zero-order states in this sequence, namely $\psi_{0\pm}$, involve the adiabatic eigenvectors $u_\pm$ in (4). The infinite series corresponding to (16) diverges, and as is well known this is associated with the existence of the transitions we seek to describe.

In sections 2 and 3 of Berry (1990a) it is shown that to lowest order in ε the first-order perturbation solution of the Schrödinger equation satisfied by $c_{n\pm}(w)$ is

$$c_{n-}(w) \approx -i\varepsilon^n \int_{-\infty}^{w} dw' \exp\left\{ -i\frac{w'}{\varepsilon} \right\} u_-^{\mathrm{T}}(w') \cdot u_{n+1,+}(w') \tag{17}$$

where T denotes the transpose. Therefore we require $u_{n+1,+}(w)$, which we find by expanding in the complete set $u_\pm(w)$, that is

$$u_{n,+}(w)=a_n(w)u_+(w)+b_n(w)u_-(w) \tag{18}$$

and substituting (16) (with $n=\infty$) into (2). This gives

$$b_n=2\frac{a_n'}{\theta'} \tag{19}$$

and the recurrence relation

$$a_n'=-\mathrm{i}\left[\tfrac{1}{4}\theta'^2 a_{n-1}+a_{n-1}''-\frac{\theta''}{\theta'}a_{n-1}'\right] \qquad (a_0(w)=1,\quad a_{n>0}(-\infty)=0) \tag{20}$$

Thus the first-order transition probability in the nth superadiabatic basis is

$$P_n\approx\left|2\mathrm{i}\varepsilon^n\int_{-\infty}^{\infty}\mathrm{d}w\,\frac{a_{n+1}'(w)}{\theta'(w)}\exp\left\{-\mathrm{i}\frac{w}{\varepsilon}\right\}\right|^2. \tag{21}$$

Just as with the adiabatic basis (cf (13) with $c_+=1$), P depends on singularities w_c of the integrand in the lower half-plane. Therefore it is necessary to solve (20) for the coefficients a_n near w_c, where (section 4) θ' has the form (12). Thus we must solve

$$a_n'=\mathrm{i}\left[\frac{\gamma^2}{4(w-w_c)^2}a_{n-1}-a_{n-1}''-\frac{1}{w-w_c}a_{n-1}'\right] \qquad (a_0(w)=1,\quad a_{n>0}(-\infty)=0) \tag{22}$$

The exact solution is

$$a_n(w)=\frac{\mathrm{i}^n(n-1-\frac{1}{2}\gamma)!(n-1+\frac{1}{2}\gamma)!}{(w-w_c)^n(-1-\frac{1}{2}\gamma)!(-1+\frac{1}{2}\gamma)!n!} \qquad (w\approx w_c) \tag{23}$$

(Regarded as an approximate solution of (20), this has fractional error of order $w-w_c$.) With (23), we obtain, from (21),

$$P_n\approx A_n^2\exp\left\{-2\frac{|\mathrm{Im}\,w_c|}{\varepsilon}\right\} \tag{24}$$

where

$$A_n=2\pi\frac{(n-\frac{1}{2}\gamma)!(n+\frac{1}{2}\gamma)!}{n!^2(-\frac{1}{2}\gamma)!(-1+\frac{1}{2}\gamma)!}=2\sin\{\tfrac{1}{2}\pi\gamma\}\frac{(n-\frac{1}{2}\gamma)!(n+\frac{1}{2}\gamma)!}{n!^2}.$$

In the adiabatic basis $n=0$, the prefactor is $A_0=\pi\gamma$, and (24) reproduces the incorrect result (14). As n increases, the prefactor renormalises onto $2\sin\{\pi\gamma/2\}$, giving the transition probability

$$P\approx P_\infty=4\sin^2\{\tfrac{1}{2}\pi\gamma\}\exp\left\{-2\frac{|\mathrm{Im}\,w_c|}{\varepsilon}\right\} \tag{25}$$

This result could also have been obtained by resumming the divergent tail of the infinite series corresponding to (16) (Berry 1990b).

4. Complex singularities

The universal form (12) occurs when $X(t)$ and $Z(t)$ have identical leading singularities at $t=t_c$ which give cancelling contributions to the energy $E(t)$. A sufficiently general form is

$$\begin{aligned} X(t) &= f(t-t_c)(1+A(t-t_c)^s+\ldots) \\ Z(t) &= \pm \mathrm{i} f(t-t_c)(1+B(t-t_c)^s+\ldots) \qquad s>0. \end{aligned} \tag{26}$$

Thus

$$E^2(t) = 2[f(t-t_c)]^2(t-t_c)^s(A-B+\ldots) \tag{27}$$

and, from (8),

$$w-w_c = 2\sqrt{2(A-B)}\int_0^{t-t_c} \mathrm{d}\tau\, f(\tau)\tau^{s/2}+\ldots. \tag{28}$$

We assume that the integral converges; there are no other restrictions on the form of $f(\tau)$.

Before proceeding, we make several remarks about this formulation. First, a simple zero in E^2 arises with f constant (i.e. not singular at all) and $s=1$; this case is generic in not requiring any conspiracy of singularities in X and Z. Second, some of the singular cases can be made generic by considering a family of Hamiltonians depending on several parameters, and varying these. Third, the cancellation of leading singularities need not imply that E has a zero; from (27), E can be constant at t_c, or diverge there.

Now we must calculate the central quantity $\theta'(w)$ near the singularity w_c. From (3) and (8),

$$\theta' = \frac{\cos^2\theta}{2E}\frac{\mathrm{d}}{\mathrm{d}t}\tan\theta = -\frac{Z^2}{2E^{3/2}}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{X}{Z}\right). \tag{30}$$

Substituting (26), we find

$$\begin{aligned} \theta' &= \frac{\pm \mathrm{i}s}{4\sqrt{2(A-B)}(t-t_c)^{s/2+1}f(t-t_c)}(1+\ldots) \\ &= \frac{\pm \mathrm{i}s}{2(w-w_c)}\frac{\int_0^{t-t_c}\mathrm{d}\tau\, f(\tau)\tau^{s/2}}{(t-t_c)^{s/2+1}f(t-t_c)}(1+\ldots). \end{aligned} \tag{31}$$

This indeed has the form (12), with the constant given by

$$\gamma = \mp\tfrac{1}{2}s\lim_{\tau\to 0}\frac{\int_0^\tau \mathrm{d}\tau\, f(\tau)\tau^{s/2}}{f(\tau)\tau^{s/2+1}} \tag{32}$$

whenever the limit exists.

A class that includes all interesting Hamiltonians we know is

$$f(\tau) = C\tau^r(1+\ldots) \tag{33}$$

for which

$$\gamma = \mp \frac{s}{2r+s+2}. \tag{34}$$

Thus the adiabatic transition probability (25) is

$$P_\infty = 4 \sin^2\left\{\frac{\pi s}{2(2r+s+2)}\right\} \exp\left\{-2\frac{|\mathrm{Im}\, w_c|}{\varepsilon}\right\}. \tag{35}$$

Transition probabilities must be invariant under arbitrary transformations to new time variables and orthogonal transformations to new quantum reference frames, that is under

$$t \to t'(t) \tag{36a}$$

$$\begin{Bmatrix} X(t) \\ Z(t) \end{Bmatrix} \to \begin{Bmatrix} X'(t) \\ Z'(t) \end{Bmatrix} \equiv \begin{Bmatrix} X(t)\cos\phi + Z(t)\sin\phi \\ -X(t)\sin\phi + Z(t)\cos\phi \end{Bmatrix} \tag{36b}$$

i.e.

$$\theta(t) \to \theta'(t) \equiv \theta(t) + \phi.$$

In appendix A we show that (34) indeed enjoys these invariance properties.

It should be emphasised that although (26), in which $X(t)$ and $Z(t)$ have the same leading singularities at $t = t_c$, generates the universal simple-pole formula (12), it represents a class of special situations. It is not difficult to find cases where the singularity of θ' is not a simple pole. For example, if $X(t) = B(t-t_c)^\mu$, $Z(t) = 1 + A(t-t_c)$, then $\theta' \sim (w-w_c)^{\mu-1}$ if $\mu > 0$, and $(w-w_c)^{(-1-2\mu)/(\mu+1)}$ if $\mu < 0$, with coefficients depending on β. In such nonuniversal cases, the prefactor in P depends on ε, and there is probably no simple general theory.

5. Examples

In the familiar Landau–Zener case,

$$X_{LZ} = 1 \qquad Z_{LZ} = t \qquad \text{i.e. } E^2 = 1 + t^2 \tag{37}$$

The form (26) is obtained in the lower half-plane by expanding about the simple zero of E^2 at $t_c = -\mathrm{i}$, and it is easy to see that $f =$ constant and (because Z deviates linearly from its value at t_c) $s = 1$, so $r = 0$ in (33) and (34) gives $\gamma = 1/3$. Thus the prefactor is unity and the adiabatic transition probability is

$$P_{\infty LZ} = \exp\left\{-\frac{\pi}{\varepsilon}\right\} \tag{38}$$

Next, consider the Hamiltonian H_A, defined in (10). Again $t_c = -\mathrm{i}$, and (8) gives $w_c = -2\mathrm{i}$. Now $f = 1/\sqrt{(1+t^2)}$, so the singularity in X and Z is a square root branch

point, with $r=-1/2$ in (33), and (because Z deviates linearly from its value at t_c) $s=1$. Thus $\gamma=1/2$ and the adiabatic transition probability is

$$P_{\infty A}=2\exp\left\{-\frac{4}{\varepsilon}\right\} \tag{39}$$

The invariance under time reparameterisation is nicely illustrated by the transformation

$$t\to\sinh t \tag{40}$$

(suggested by Dr Alain Joye). This preserves the structure of (2) and gives

$$X_A=1 \qquad Z_A=\sinh t \qquad \text{i.e. } E^2=\cosh^2 t. \tag{41}$$

Now the form (26) is obtained by expanding about the double zero of E^2 at $t_c=-i\pi/2$, giving $r=0$ in (33) and $s=2$. These are different values from those generated by the formulae in (10), but of course refer to the same Hamiltonian H_A and so generate the same γ and the same transition probability.

Our last example is the Hamiltonian H_B, defined in (10). Again $t_c=-i$, and (8) gives $w_c=-2i$. Now $f=\operatorname{sech} t$, so the singularity in X and Z is a simple pole, with $r=-1$ in (33), and (because Z deviates quadratically from its value at t_c) $s=2$. Thus $\gamma=1$ and the adiabatic transition probability is

$$P_{\infty B}=4\exp\left\{-\frac{4}{\varepsilon}\right\}. \tag{42}$$

Each of these three Hamiltonians has a different status in adiabatic theory. H_{LZ} is exactly solvable, and the solution (Zener 1932) shows that the adiabatic formula (38) is in fact exact. H_A seems to have no exact solution, and we suppose that the formula (39) is the first term in an adiabatic expansion in powers of ε. This is supported by numerical exploration. (Computational solution of (2) for small ε is not trivial; the method we employed is outlined in appendix B.) H_B does have an exact solution

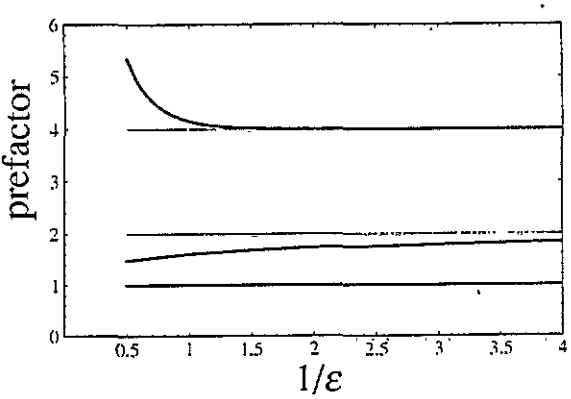

Figure 1. Prefactors (thick lines) multiplying the leading exponential in the transition probability, as functions of the adiabatic parameter ε, for the Hamiltonians H_{LZ} (equation (36)), H_A and H_B (equation (10)). The LZ prefactor is exactly unity, and the A and B prefactors are asymptotic to 2 and 4 respectively.

(described by Suominen and Garraway 1992), namely

$$P_B=\frac{1}{\sinh^2\left(\dfrac{2}{\varepsilon}\right)}=\frac{4\exp\left\{-\dfrac{4}{\varepsilon}\right\}}{\left(1-\exp\left\{-\dfrac{4}{\varepsilon}\right\}\right)^2}=P_{\infty B}\left(1+2\exp\left\{-\frac{4}{\varepsilon}\right\}+\ldots\right). \tag{43}$$

Therefore the error is exponentially small, and results not from an adiabatic expansion associated with the singularity at $w_c=-2i$ but from contributions associated with other singularities (Suominen 1992).

Figure 1 shows the exact prefactors for the three Hamiltonians as functions of ε, indicating clearly the considerably lower accuracy of the adiabatic approximation for H_A.

Acknowledgment

We are grateful to Dr Alain Joye for sending us his different and independent derivation of the prefactors.

Appendix A

First we show that the formula (34) for γ, and hence the adiabatic transition probability (35), is invariant under (36*a*), i.e. time reparameterisation. From (2) and (3), the new Hamiltonian involves

$$\begin{Bmatrix} X'(t') \\ Z'(t') \end{Bmatrix}=\frac{\mathrm{d}t}{\mathrm{d}t'}\begin{Bmatrix} X(t(t')) \\ Z(t(t')) \end{Bmatrix}. \tag{A1}$$

Now suppose

$$t-t_c\propto(t'-t_c')^{\mu} \tag{A2}$$

The quantities in (26) and (33) rescale as

$$s\to s'=\mu s \qquad r\to r'=r\mu+\mu-1 \tag{A3}$$

and this leaves (34) invariant.

Now we demonstrate the invariance under (36*b*), i.e. quantum orthogonal transformation. This changes (26) to

$$\begin{aligned} X'(t)&=\exp\{\mathrm{i}\phi\}f(t-t_c)[1+(t-t_c)\exp\{-\mathrm{i}\phi\}(A\cos\phi+\mathrm{i}B\sin\phi)] \\ Z'(t)&=\mathrm{i}\exp\{\mathrm{i}\phi\}f(t-t_c)[1+(t-t_c)\exp\{-\mathrm{i}\phi\}(B\cos\phi+\mathrm{i}A\sin\phi)]. \end{aligned} \tag{A4}$$

Clearly the form of (26) is preserved, with

$$\begin{aligned} &f(t-t_c)\to f'(t-t_c)=\exp\{\mathrm{i}\phi\}f(t-t_c) \\ &A\to A'=A\cos\phi+\mathrm{i}B\sin\phi \\ &B\to B'=B\cos\phi+\mathrm{i}A\sin\phi. \end{aligned} \tag{A5}$$

Appendix B

The numerical solution of (2) for small ε, given a Hamiltonian specified by functions $X(t)$, $Z(t)$ is complicated by the fact that the desired final transition amplitude is an exponentially small quantity emerging from rapid oscillations that are much larger. This numerical instability can be reduced by solving the Schrödinger equation not in the original basis, or the adiabatic basis defined by (4) and (5), but in one of the superadiabatic bases. As explained by Berry (1990a) and Lim and Berry (1991), the optimal basis would be the one whose order is the nearest integer to $|w_c|/\varepsilon$ (because in the nth basis the oscillations of the transition amplitude $c_{n-}(t)$ are of order $\varepsilon^{n+1}/n!$).

However, it is not necessary to use the optimal basis; in the computations with H_A illustrated in figure 1, only the first-order ($n=1$) superadiabatic basis was employed, and this was dramatically superior to the ordinary adiabatic basis ($n=0$).

For numerical purposes the most convenient sequence of superadiabatic bases is not that defined by the perturbation expansion (16) (although this is useful for theoretical purposes), but that generated by adiabatic iteration Berry (1987). In this procedure, the system is transformed to a basis specified by the eigenstates of the instantaneous Hamiltonian, and the process is repeated. If we define

$$x_0(t) \equiv \frac{2X(t)}{\varepsilon} \qquad z_0(t) \equiv \frac{2Z(t)}{\varepsilon} \tag{B1}$$

then with a particular choice of phases the successive Hamiltonians are determined by

$$\begin{aligned} x_{n+1}(t) &\equiv \frac{x_n(t)\dot{z}_n(t) - z_n(t)\dot{x}_n(t)}{x_n^2(t) + z_n^2(t)} \\ z_{n+1}(t) &\equiv \sqrt{x_n^2(t) + z_n^2(t)}\,. \end{aligned} \tag{B2}$$

These functions can easily be found by repeated differentiation.

It is also convenient (see also Suominen 1992) to solve not the Schrödinger equation but the equivalent real equation for the spin vector (expectation value of the vector of Pauli spin matrices) on the Bloch sphere. For the nth superadiabatic basis this is

$$\begin{aligned} &\dot{\boldsymbol{S}}_n(t) = \boldsymbol{r}_n(t) \wedge \boldsymbol{S}_n(t) \\ &\text{where} \\ &\boldsymbol{S}_n(t) \equiv \{S_{n1}(t),\, S_{n2}(t),\, S_{n3}(t)\} \\ &\boldsymbol{r}_n(t) \equiv \{x_n(t),\, 0,\, z_n(t)\} \qquad \boldsymbol{S}_n(0) = \{0,\, 0,\, 1\} \end{aligned} \tag{B3}$$

and we used the Runge–Kutta method for its numerical solution. In this formulation, the transition probability is

$$P = \tfrac{1}{2}[1 - S_{n3}(+\infty)]. \tag{B4}$$

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