Geometric amplitude factors in adiabatic quantum transitions

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The exponentially small probability of transition between two quantum states, induced by the slow change over infinite time of an analytic hamiltonian $\hat{H} = \boldsymbol{H}(\delta t)\cdot\hat{\boldsymbol{S}}$ (where δ is a small adiabatic parameter and $\hat{\boldsymbol{S}}$ is the vector spin-$\frac{1}{2}$ operator), contains an additional factor $\exp\{\Gamma_g\}$ of purely geometric origin (that is, independent of δ and $\hbar$). For Γ_g to be non-zero, $\hat{H}$ must be complex hermitian rather than real symmetric, and the hamiltonian curve $\boldsymbol{H}(\tau)$ must not lie in a plane through the origin nor be a helix identical (up to rigid motion) with its time reverse. An expression is given for Γ_g, as an integral from the real t axis to the complex time of degeneracy of the two states. Explicit examples are given. The geometric effect could be observed in experiments with spinning particles.

1. Introduction

It is well known that the state of a quantum system forced round a cycle by slow (adiabatic) change in its governing hamiltonian will return with its phase changed, by an amount that is in part purely geometric (Berry 1984; Shapere & Wilczek 1989). It is also known (Garrison & Wright 1988) that if the evolution is dissipative (non-unitary) the geometric 'phase' can be complex, so there can be a geometric change in the amplitude, and hence in the probability of still being in the initial state at the end of the cycle.

Here I draw attention to a different geometric effect, also an amplitude but one which can occur in unitary evolutions, that is in quantum systems without dissipation. This exists in the transition amplitude at $t \to +\infty$ for finding the system in a state different from the adiabatic eigenstate in which it was prepared at $t \to -\infty$. The transition is driven by the time dependence of the hermitian hamiltonian $\hat{H}(\delta t)$ where δ is an adiabatic parameter that can be made small. Transitions are exponentially weak (i.e. of order $\exp\{-1/\delta\}$), but for certain kinds of time dependence (for which $\hat{H}$ is essentially complex hermitian rather than real symmetric) there is an additional exponential factor which is of order unity and geometric in character.

The simplest manifestations of the geometric amplitude occur in two-state systems, to which we restrict attention here. In terms of 'slow time' $\tau \equiv \delta t$, the hamiltonian is

$$\hat{H}(\tau) = \boldsymbol{H}(\tau)\cdot\hat{\boldsymbol{S}} \equiv \begin{pmatrix} Z(\tau) & X(\tau) - \mathrm{i}Y(\tau) \\ X(\tau) + \mathrm{i}Y(\tau) & -Z(\tau) \end{pmatrix}$$

$$= H(\tau)\begin{pmatrix} \cos\theta(\tau) & \sin\theta(\tau)\exp\{-\mathrm{i}\phi(\tau)\} \\ \sin\theta(\tau)\exp\{+\mathrm{i}\phi(\tau)\} & -\cos\theta(\tau) \end{pmatrix} \quad (1)$$

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involving the vector spin-$\frac{1}{2}$ operator $\hat{\boldsymbol{S}}$ and the *hamiltonian vector* $\boldsymbol{H}$ with cartesian components X, Y, Z and polar components H, θ, ϕ. Crucial will be the geometry of the *hamiltonian curve* drawn by $\boldsymbol{H}(\tau)$ between $-\infty < \tau < +\infty$; this curve need not be closed. We assume that X, Y and Z are analytic functions of τ in a strip including the whole real axis. One realization of $\hat{H}$ is a spin-$\frac{1}{2}$ particle in a slowly changed magnetic field $\boldsymbol{H}$.

At any instant, $\hat{H}(t)$ has two eigenstates, $|u_+(\tau)\rangle$ and $|u_-(\tau)\rangle$, with eigenvalues

$$E_{\pm}(\tau) = \pm H(\tau) = \pm\surd(X^2(\tau)+Y^2(\tau)+Z^2(\tau)). \tag{2}$$

We assume that H is non-zero for all real τ, i.e. that there are no degeneracies of these instantaneous eigenstates. Consider a system whose initial state is $|u_+(-\infty)\rangle$. In the limit $\delta = 0$ (infinitely slow change) the adiabatic theorem (Born & Fock 1928; see also Messiah 1962) guarantees that the state will subsequently be $|u_+(\tau)\rangle$, apart from a phase, and this is true in particular for the final state $|u_+(+\infty)\rangle$. Here our interest is focused on the weak transitions that occur when δ is small but not zero. We seek the probability P that the system will finally be found in the state $|u_-(+\infty)\rangle$.

Such 'adiabatic transitions' are associated with *complex degeneracies* of the instantaneous eigenvalues, that is complex times $\tau = \tau_c$ for which

$$H(\tau_c) = 0 \tag{3}$$

(Dykhne 1962; Davis & Pechukas 1976; Hwang & Pechukas 1977). These roots come in conjugate pairs; here the important τ_c is the root closest to the real axis in the lower half-plane (we assume that the analyticity strip of $\hat{H}$ – that is, of $X(\tau)$, $Y(\tau)$, $Z(\tau)$ – includes this root). The new effect to be described here arises out of the analytic continuation to τ_c of the hamiltonian curve, and is non-zero only when the curve does not lie in a plane through $\boldsymbol{H} = 0$.

The formula for P (including its geometric part) can be derived in two ways. It is instructive to present both derivations (§§2 and 3). Some general properties of the geometric amplitude are given in §4, and some explicit examples in §5.

2. Derivation by parallel transport

In the adiabatic approximation, the evolving state, satisfying

$$\mathrm{i}\hbar\, \mathrm{d}_t|\psi(t)\rangle = \hat{H}(\delta t)|\psi(t)\rangle \tag{4}$$

is given by

$$|\psi(t)\rangle \approx \exp\left\{-\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t\, H(\delta t)\right\}|u_+(\delta t)\rangle. \tag{5}$$

Here $|u_+(\tau)\rangle$ satisfies

$$\hat{H}(\tau)|u_+(\tau)\rangle = +H(\tau)|u_+(\tau)\rangle, \tag{6}$$

where from (4) in the adiabatic limit the phase of $|u_+(\tau)\rangle$ is fixed by the parallel transport requirement (Berry 1984)

$$\langle u_+|\dot{u}_+\rangle = 0 \tag{7}$$

(here and hereafter an overdot denotes a τ derivative).

The explicit solution of (6) and (7) with the hamiltonian (1) is

$$|u_+(\tau)\rangle = \begin{pmatrix} \cos\{\tfrac{1}{2}\theta(\tau)\}\exp\{-\tfrac{1}{2}\mathrm{i}\phi(\tau)\} \\ \sin\{\tfrac{1}{2}\theta(\tau)\}\exp\{+\tfrac{1}{2}\mathrm{i}\phi(\tau)\} \end{pmatrix} \exp\{\mathrm{i}\mu(\tau)\}, \tag{8}$$

where

$$\mu(\tau) = \frac{1}{2}\int_0^\tau \mathrm{d}\tau' \dot{\phi}\cos\theta = \frac{1}{2}\int_0^\tau \mathrm{d}\tau' \frac{(X\dot{Y}-Y\dot{X})Z}{(X^2+Y^2)\sqrt{(X^2+Y^2+Z^2)}} \tag{9}$$

(as in (5) we have chosen the arbitrary phase origin at $\tau = 0$). If the hamiltonian curve is closed, (9) gives the familiar geometric phase anholonomy: $\mu(+\infty)-\mu(-\infty)$ is the solid angle subtended by the curve at the origin $\boldsymbol{H} = 0$.

For small δ, the amplitude for being in the other state $|u_-\rangle$ is obtained by analytic continuation of (5) round τ_c (Davis & Pechukas 1976), for the following reason. If, as we assume, τ_c is a simple zero of $X^2+Y^2+Z^2$, it is also a branch point of $H(\tau)$, connecting two sheets representing $|u_+\rangle$ and $|u_-\rangle$ and around which $|u_+\rangle$ transforms into $|u_-\rangle$. For small δ the final transition probability is then the product of two contributions:

$$P \equiv |\langle u_-(+\infty)|\psi(+\infty)\rangle|^2 \approx \exp\{-\Gamma_\mathrm{d}\}\exp\{+\Gamma_\mathrm{g}\}. \tag{10}$$

Γ_d is the familiar 'dynamical' exponent from the continuation of the integral in (5):

$$\Gamma_\mathrm{d} = -\frac{4}{\hbar\delta}\mathrm{Im}\int_0^{\tau_c} \mathrm{d}\tau\, H(\tau) = \frac{4}{\hbar\delta}\left|\mathrm{Im}\int_0^{\tau_c}\mathrm{d}\tau\, H(\tau)\right| \tag{11}$$

(the factor 4 is the product of two 2s: one because the continuation runs down to τ_c and back, and one because P is the square of a probability amplitude). Γ_g, the contribution of interest here, is a geometric exponent, generated by the analytic continuation of the phase $\mu(\tau)$ in (9):

$$\Gamma_\mathrm{g} = -2\,\mathrm{Im}\int_0^{\tau_c}\mathrm{d}\tau\dot{\phi}\cos\theta. \tag{12}$$

The formula (12) is our main result. Note that Γ_g, unlike Γ_d, is independent of δ and therefore also independent of $\hbar$. It depends only on the analytic continuation of the hamiltonian curve; that is why it is geometric. If we cut the τ plane between the complex degeneracies τ_c and τ_c^*, we can write Γ_g as the circuit integral

$$\Gamma_\mathrm{g} = -\tfrac{1}{2}\mathrm{Im}\oint \mathrm{d}\tau\dot{\phi}\cos\theta = -\tfrac{1}{2}\mathrm{Im}\oint \mathrm{d}\phi\cos\theta \tag{13}$$

around the cut. It is tempting to transform this by Stokes's theorem into the integral of a 2-form, and interpret Γ_g as a solid angle in complexified $\boldsymbol{H}$ space, by analogy with the geometric phase for cycles with real $\boldsymbol{H}$. However, this gives little additional insight because the deformability of the integration contour in (13), arising from the analytic structure of the problem, means that the 2-form must vanish except on the cut. (This contrasts with the dissipative phenomena considered by Garrison & Wright (1988), in which a complex solid angle does play a useful part.)

It should be remarked here that the 'circuit-dependent adiabatic phase' discussed by Coveney *et al.* (1988) is not geometric but rather an ordinary dynamical phase, associated with Γ_d.

3. Derivation by transformation to rotating frame

The hamiltonian (1) can be made real symmetric by eliminating its imaginary part through the transformation

$$|\psi\rangle = \hat{U}(\tau)|\psi'\rangle \equiv \begin{pmatrix} \exp\{-\tfrac{1}{2}\mathrm{i}\phi(\tau)\} & 0 \\ 0 & \exp\{\tfrac{1}{2}\mathrm{i}\phi(\tau)\} \end{pmatrix}|\psi'\rangle. \tag{14}$$

$|\psi'\rangle$ satisfies a Schrödinger equation in which $\hat{H}$ is replaced by

$$\begin{aligned} \hat{H}'(\tau) &= \hat{U}^{+}\hat{H}\hat{U} - \mathrm{i}\hbar\delta\hat{U}^{+}\dot{\hat{U}} \\ &= \begin{pmatrix} Z-\tfrac{1}{2}\hbar\delta\dot{\phi} & \surd(X^2+Y^2) \\ \surd(X^2+Y^2) & -(Z-\tfrac{1}{2}\hbar\delta\dot{\phi}) \end{pmatrix} \\ &= \begin{pmatrix} Z' & X' \\ X' & -Z' \end{pmatrix}. \end{aligned} \tag{15}$$

Since $\hat{H}'$ is real (i.e. $Y' = 0$), the analogue μ' of μ in (9) vanishes and there appears to be no geometric contribution. But the transformation to (15) has altered the adiabatic energies, to

$$\begin{aligned} E'_{\pm}(\tau) &= \pm\surd([X'(\tau)]^2+[Z'(\tau)]^2) \\ &= \pm\surd[(Z-\tfrac{1}{2}\hbar\delta\dot{\phi})^2+X^2+Y^2]. \end{aligned} \tag{16}$$

Thus the transition probability, now apparently entirely dynamical, is modified and we have, on expanding the exponent to the lowest-order non-vanishing in δ,

$$\begin{aligned} P \approx \exp\{-\Gamma'_{\mathrm{d}}\} &= \exp\left\{\frac{4}{\hbar\delta}\mathrm{Im}\int_0^{\tau_c}\mathrm{d}\tau\, E'_{+}(\tau)\right\} \\ &\approx \exp\left\{-\frac{4}{\hbar\delta}\left|\mathrm{Im}\int_0^{\tau_c}\mathrm{d}\tau\, H(\tau)\right| - 2\,\mathrm{Im}\int_0^{\tau_c}\mathrm{d}\tau\frac{\dot{\phi}Z}{H}\right\}, \end{aligned} \tag{17}$$

which is exactly the same as our previous (10)–(12).

Earlier (Berry 1987), I have discussed in a more general context the interpretational ambiguity exemplified by these two derivations, in which the geometric exponent Γ_{g} appears to be generated by parallel transport or by dynamics. Of course, the ambiguity extends only to the derivations, and not the result, which is the same in both cases, and unambiguously geometric.

4. General properties of the geometric exponent

The first property is that Γ_{g} vanishes, i.e. there is no geometric factor in (10), for any hamiltonian curve $\boldsymbol{H}(\tau)$ confined to a plane including the origin $\boldsymbol{H} = 0$. To see this, observe that by rotation of axes the plane containing the curve can be chosen with constant longitude ϕ. Therefore $\dot{\phi}$ vanishes for real τ and so does its analytic continuation in (12). (It is an interesting and tricky exercise to prove this property without rotation of axes; I do not give the argument here.)

The second property is that if the hamiltonian curve is traversed backwards (that is if $\boldsymbol{H}(\tau)$ is replaced by $\boldsymbol{H}(-\tau)$), Γ_{g} changes sign. This follows from the fact that the backward traversal causes $\dot{\phi}$ in (12) to change sign. Note that this transformation does not reverse Γ_{d}.

The third property is that for the opposite transition, from $|u_-\rangle$ to $|u_+\rangle$, Γ_g, like Γ_d, does not change sign. This can be seen most easily by repeating the argument leading to (17), with E_- replacing E_+. More fundamentally, the reason for the property is that the evolution operator associated with $\hat{H}$ is unitary and so its off-diagonal elements are equal in modulus.

The fourth property, which follows from the second, is that Γ_g vanishes for any reversible hamiltonian curve, that is any curve which can be rigidly rotated into itself about an axis through $\boldsymbol{H} = 0$. To see this analytically, let the rotation axis be the X axis, and let the curve cross it at $\tau = 0$. Then the symmetry under discussion is

$$H(-\tau) = H(\tau), \quad \theta(-\tau) = \pi - \theta(\tau), \quad \phi(-\tau) = -\phi(\tau). \tag{18}$$

Since $H(\tau)$ is even, any single zero τ_c in the lower half-plane and nearest the real axis must lie on the imaginary axis (we ignore the case where the nearest τ_c form pairs with opposite real parts and the same imaginary part). Thus in (12) $\mathrm{d}\tau$ is imaginary. We also have, from (18), that $\cos\theta(\tau)$ is odd and hence imaginary on the imaginary axis, and $\dot{\phi}$ is even and hence real on the imaginary axis. Taken together, these results imply that $\mathrm{d}\tau\,\dot{\phi}\cos\theta$ is real, so Γ_g does indeed vanish for reversible curves.

5. Twisted Landau–Zener models

These have hamiltonian vector

$$\boldsymbol{H}(\tau) = (\Delta\cos\phi(\tau), \Delta\sin\phi(\tau), A\tau) \tag{19}$$

so the hamiltonian curve lies on a cylinder centred on the Z axis. The familiar Landau–Zener model (Zener 1932) is the special case $\phi = 0$. For any $\phi(\tau)$, we have

$$H^2(\tau) = A^2\tau^2 + \Delta^2 \tag{20}$$

so the complex degeneracy is at

$$\tau_c = -\mathrm{i}\Delta/|A|. \tag{21}$$

This generates the dynamical exponent

$$\begin{aligned}\Gamma_d &= -\frac{4}{\hbar\delta}\,\mathrm{Im}\int_0^{-\mathrm{i}\Delta/|A|} \mathrm{d}\tau\,\surd(\Delta^2 + A^2\tau^2) \\ &= \frac{4}{\hbar\delta}\int_0^{\Delta/|A|} \mathrm{d}y\,\surd(\Delta^2 - A^2y^2) = \frac{\pi\Delta^2}{\hbar\delta|A|},\end{aligned} \tag{22}$$

which is independent of the twist $\phi(\tau)$ and therefore the same as in the ordinary Landau–Zener case.

For the geometric exponent, we need

$$\cos\theta = Z/H = A\tau/\surd(A^2\tau^2 + \Delta^2). \tag{23}$$

Now (12) gives

$$\begin{aligned}\Gamma_g &= -2\,\mathrm{Im}\int_0^{-\mathrm{i}\Delta/|A|} \mathrm{d}\tau\,\dot{\phi}\frac{A\tau}{\surd(A^2\tau^2 + \Delta^2)} \\ &= 2A\int_0^{\Delta/|A|} \mathrm{d}y\,\frac{y}{\surd(\Delta^2 - A^2y^2)}\,\mathrm{Im}\,\dot{\phi}(-\mathrm{i}y).\end{aligned} \tag{24}$$

If ϕ is an odd function of τ, Γ_g vanishes, thereby exemplifying the fourth property

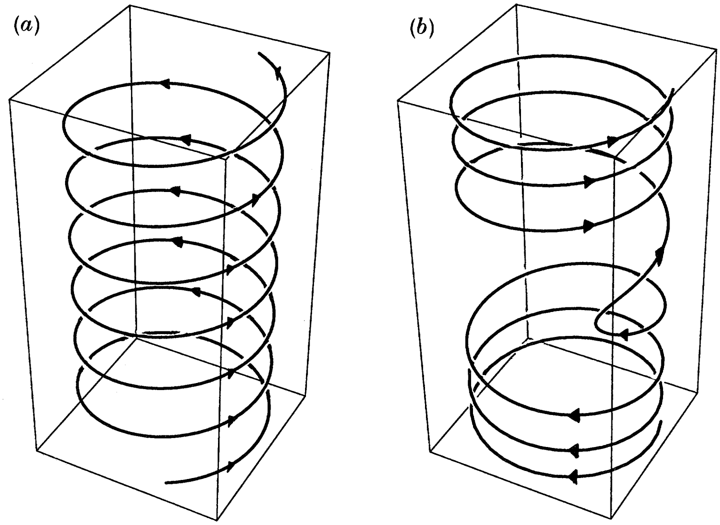

Figure 1. Hamiltonian curves in the twisted Landau–Zener model (19). (a) Uniform helix $\phi(\tau) = \tau$, for which the geometric exponent Γ_g vanishes because the curve is identical (after a rotation) to its time-reverse (in which $\phi(\tau) = -\tau, Z(t) = -A\tau$. (b) Winding–unwinding helix $\phi(\tau) = B\tau^2$, for which Γ_g (equation (27)) does not vanish because the curve is the mirror image of its reverse.

in §4 (it is easy to confirm that the hamiltonian (19) possesses the symmetries (18) when ϕ is odd). In particular, $\Gamma_g = 0$ for $\phi = \tau$, that is when the hamiltonian curve is a uniformly wound helix (figure 1a). The simplest non-trivial case is

$$\phi = B\tau^2, \tag{25}$$

which is a helix that winds for $-\infty < \tau < 0$ and then unwinds (figure 1b). Rather than being reversible (as in (18)), this curve's reversal generates its mirror image. From (24) we have

$$\Gamma_g = -4BA \int_0^{\Delta/|A|} dy \frac{y^2}{\surd(\Delta^2 - A^2y^2)} = -\pi \frac{B\Delta^2}{A^2} \operatorname{sgn}(A). \tag{26}$$

The fact that this is an odd function of both A and B exemplifies the second property in §4, because changing the sign of A or B is equivalent to reversing the hamiltonian curve (for A this follows immediately from (19) with (25); for B it follows after a rigid rotation of the curve).

It so happens that for the particular choice (25) the transition probability can be found exactly (i.e. not just in the adiabatic approximation), thereby affording a check of (26). The trick is to rotate the hamiltonian, by (14), into (15), which then becomes the ordinary Landau–Zener hamiltonian with Z replaced by

$$Z' = Z - \tfrac{1}{2}\hbar\delta\dot{\phi} = A\tau(1 - \hbar\delta B/A). \tag{27}$$

Now the exact twisted Landau–Zener solution is obtained simply by renormalizing A in the ordinary Landau–Zener solution to $A(1-\hbar\delta B/A)$:

$$P = \exp\left\{-\frac{\pi\Delta^2}{\hbar\delta|A(1-\hbar\delta B/A)|}\right\}. \tag{28}$$

The geometric exponent (26) emerges from the first-order correction in the expansion of the exponent in powers of δ; this correction is of zero order in δ and $\hbar$. Of course

(28) is also the transition probability from $|u_-\rangle$ to $|u_+\rangle$, thereby exemplifying the third property in §4.

6. Concluding remarks

The general arguments presented here are valid in the adiabatic limit $\delta \to 0$. Then the geometric amplitude factor, with exponent Γ_g given by (12), multiplies a dynamical factor which is exceedingly small because its exponent Γ_d, given by (11), is negative and of order $1/\delta$. If, however, this small transition probability could be measured, it would be possible to identify the geometric contribution. There are at least two ways in which this could be done. One is to vary the speed δ with which the hamiltonian curve is traversed, and plot $\log(P^{-1})$ against δ^{-1}: Γ_g is then the intercept, on the ordinate, of the large-δ^{-1} asymptote. The other way is to measure P with $\hat{H}$ and the reversed $\hat{H}$: Γ_g is then half the logarithm of the ratio of the measured probabilities.

Finally, I ought to expand the cautionary remark that even in the adiabatic limit the results given here are valid only if the analyticity strip of the hamiltonian is wide enough to include the nearest complex degeneracies τ_c. Otherwise – that is if $\hat{H}$ itself has singularities closer to the real axis than τ_c – the asymptotic behaviour can be different from that described by (10)–(12), and difficult to determine. One example is the twisted Landau–Zener model (19) with

$$\exp\{i\phi(\tau)\} = \left(\frac{\tau^2 - 2i\Delta^2/B^2}{\tau^2 + 2i\Delta^2/B^2}\right)^{\alpha/\pi} \tag{29}$$

for which the hamiltonian curve is a helix winding through an angle α and then unwinding. This has branch points closer to the real axis than τ_c if $B > \Delta$. Another example is hamiltonian curves confined to a sphere centred on $\boldsymbol{H} = 0$. Then H is constant and there are no complex degeneracies anywhere in the plane, that is $|\mathrm{Im}\,\tau_c| = \infty$.

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References

Berry, M. V. 1984 *Proc. R. Soc. Lond.* A **392**, 45–57.
Berry, M. V. 1987 *Proc. R. Soc. Lond.* A **414**, 31–46.
Born, M. & Fock, V. A. 1928 *Z. Phys.* **51**, 165–169.
Coveney, P. V., Crothers, D. S. F. & Macek, J. H. 1988 *J. Phys.* B **21**, L165–L168.
Davis, J. P. & Pechukas, P. 1976 *J. chem. Phys.* **64**, 3129–3137.
Dykhne, A. M. 1962 *Sov. Phys. JETP* **14**, 941–943.
Garrison, J. C. & Wright, E. M. 1988 *Phys. Lett.* A **128**, 177–181.
Hwang, J.-T. & Pechukas, P. 1977 *J. chem. Phys.* **67**, 4640–4653.
Messiah, A. 1962 *Quantum mechanics*, vol. 2. Amsterdam: North-Holland.
Shapere, A. & Wilczek, F. 1989 *Geometric phases in physics*. Singapore: World Scientific.
Zener, C. 1932 *Proc. R. Soc. Lond.* A **137**, 696–702.

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Note added in proof (16 May 1990). In a preprint from the EPF–Lausanne, A. Joye, H. Kunz and Ch.-Ed. Pfister present, without elaboration, a result equivalent to (12).