Proc. R. Soc. Lond. A **414**, 31–46 (1987)
Printed in Great Britain

Quantum phase corrections from adiabatic iteration

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(*Received* 22 *April* 1987)

The phase change γ acquired by a quantum state $|\psi(t)\rangle$ driven by a hamiltonian $H_0(t)$, which is taken slowly and smoothly round a cycle, is given by a sequence of approximants $\gamma^{(k)}$ obtained by a sequence of unitary transformations. The phase sequence is not a perturbation series in the adiabatic parameter ϵ because each $\gamma^{(k)}$ (except $\gamma^{(0)}$) contains ϵ to infinite order. For spin-$\frac{1}{2}$ systems the iteration can be described in terms of the geometry of parallel transport round loops C_k on the hamiltonian sphere. Non-adiabatic effects (transitions) must cause the sequence of $\gamma^{(k)}$ to diverge. For spin systems with analytic $H_0(t)$ this happens in a universal way: the loops C_k are sinusoidal spirals which shrink as ϵ^k until $k \sim \epsilon^{-1}$ and then grow as $k!$; the smallest loop has a size $\exp\{-1/\epsilon\}$, comparable with the non-adiabaticity.

1. Introduction

It is known (Berry 1984) that the phase of a quantum system whose hamiltonian is taken slowly round a cycle will acquire a geometric contribution, characteristic of the cycle, as well as the familiar dynamical one. The argument assumed that the instantaneous eigenstates were non-degenerate and that the adiabatic theorem could be applied. Two generalizations have removed these restrictions: Wilczek & Zee (1984) allow the instantaneous eigenstates to be degenerate (see also Segert 1987 and Mead 1987); and Aharonov & Anandan (1987) (see also Page 1987) allow the evolution to be non-adiabatic provided the system returns exactly to its initial state (apart from a phase, of course).

My purpose here is to develop a third generalization, going back to the original non-degenerate adiabatic scenario in which the system returns to its original state not exactly but in a close approximation, but now taking into account the finite rate at which the hamiltonian is changed. This leads to a technique for systematically obtaining corrections to the geometric phase. Garrison (1986) has made a start along these lines, by calculating the first phase correction in adiabatic perturbation theory. The method I shall use is not perturbative but iterative, and involves a sequence of unitary transformations chosen so as to make the hamiltonian cling ever more closely to the evolving state; it has the merit of being easy to visualize.

In §2 the phase is defined precisely and the iteration scheme described. It is shown how the phase can be interpreted as geometric or dynamical, depending on the choice of unitary transformation. The simplest non-trivial application (§3) is to a two-state (spin-$\frac{1}{2}$) system, for which the iteration can be formulated explicitly

in terms of geometry on the hamiltonian sphere. For finite slowness the evolution of the state will not be perfectly adiabatic, and as will be explained in §4 this implies the eventual divergence of the iteration scheme for the phase; for spin systems the divergence exhibits remarkable universality.

2. Iterated adiabatic anholonomy

Let the state $|\psi_0(t)\rangle$ be driven by a hamiltonian $H_0(t)$ (the suffixes denote the zeroth state of the iteration scheme to be described below). In units with $\hbar = 1$, $|\psi_0\rangle$ satisfies

$$\mathrm{i}\,|\dot{\psi}_0\rangle = H_0\,|\psi_0\rangle, \tag{1}$$

where here and hereafter time-dependences are understood where not written explicitly, and dots denote time derivatives. H_0 is taken smoothly round a cycle, i.e. $H_0(+\infty) = H_0(-\infty)$ with all derivatives vanishing as $|t| \to \infty$ (for this it suffices to take H_0 analytic in a strip including the real t axis). Let the (non-degenerate) instantaneous eigenstates of H_0 be $|n_0(t)\rangle$ with energies $E_0(n,t)$, i.e.

$$H_0\,|n_0\rangle = E_0(n)\,|n_0\rangle. \tag{2}$$

This defines the $|n_0\rangle$ up to a time-dependent phase which we make unique by demanding that

$$\langle n_0\,|\,\dot{n}_0\rangle = 0. \tag{3}$$

With this choice, the eigenstates are parallel-transported, as explained by Simon (1983). Let the system start in the nth eigenstate, i.e.

$$|\psi_0(-\infty)\rangle = |n_0(-\infty)\rangle \equiv |N\rangle. \tag{4}$$

The phase which is the object of study is now defined as

$$\gamma(n) \equiv \mathrm{Im}\,\ln\langle N|\,\psi_0(+\infty)\rangle + \int_{-\infty}^{\infty} \mathrm{d}t\,E_0(n,t). \tag{5}$$

This form of writing assumes that the integral over E_0 (which is minus the dynamical phase) converges, or can be made to converge by shifting the energy origin; if not, γ can be defined by a suitable limiting procedure. As defined by (5) the phase is more general than that which arises in the cyclic evolutions of Aharonov & Anandan (1987), because transitions may (and usually do) make $|\langle N|\,\psi_0(+\infty)\rangle| < 1$, i.e. the final state may be a superposition including states other than the original. Here, however, the emphasis is on cases where such non-adiabatic effects are small. We shall introduce a slowness parameter ϵ, entering H_0 in the combination ϵt, and regard ϵ as small. In the limit $\epsilon = 0$, γ becomes the geometric phase studied previously (Berry 1984).

Now let us follow several other authors (e.g. Avron *et al.* 1987; Anandan & Stodolsky 1987; Mead 1987) and define $U_0(t)$ as the unitary operator generating the eigenstates $|n_0(t)\rangle$ by acting on the original eigenstates $|N\rangle$, i.e.

$$|n_0(t)\rangle = U_0(t)\,|N\rangle. \tag{6}$$

Because of the parallel-transport law (3), $|n_0(+\infty)\rangle$ differs from $|N\rangle$ by a phase which is precisely the original geometric phase $\gamma_0(n)$ (anholonomy of H_0), so that

$$U_0(+\infty)\,|N\rangle = \exp\{\mathrm{i}\,\gamma_0(n)\}\,|N\rangle. \tag{7}$$

The operator U_0 naturally leads to a new representation of the evolving state $|\psi_0\rangle$ as that state $|\psi_1\rangle$ on which it must act to produce $|\psi_0\rangle$, i.e.

$$|\psi_1\rangle = U_0^\dagger\,|\psi_0\rangle. \tag{8}$$

Thus

$$\langle N\,|\,\psi_0(+\infty)\rangle = \langle N\,|\,U_0(+\infty)\,|\,\psi_1(+\infty)\rangle = \exp\{\mathrm{i}\,\gamma_0\}\,\langle N\,|\,\psi_1(+\infty)\rangle \tag{9}$$

so that the phase (5) now becomes

$$\gamma(n) = \gamma_0(n) + \mathrm{Im}\,\ln\langle N\,|\,\psi_1(+\infty)\rangle + \int_{-\infty}^{\infty} \mathrm{d}t\,E_0(n,t). \tag{10}$$

To proceed further, we need the Schrödinger equation satisfied by $|\psi_1\rangle$. This involves a hamiltonian $H_1(t)$ which differs from H_0, because the transformation U_0 is time-dependent. Thus

$$\mathrm{i}\,|\dot{\psi}_1\rangle = H_1\,|\psi_1\rangle, \tag{11}$$

where

$$H_1 = U_0^\dagger H\,U_0 - \mathrm{i}\,U_0^\dagger \dot{U}_0. \tag{12}$$

It is not difficult to show from (2), (3) and (6) that the matrix elements of H_1 in the $|N\rangle$ representation are

$$\langle M\,|\,H_1|\,N\rangle = E_0(n)\,\delta_{MN} - \frac{\mathrm{i}\,\langle m_0\,|\dot{H}_0|\,n_0\rangle}{E_0(n) - E_0(m)}(1-\delta_{MN}). \tag{13}$$

The simplest adiabatic approximation is to neglect the off-diagonal elements on the grounds that $\dot{H}_0$ is of order ϵ. Then (11) gives

$$|\psi_1(t)\rangle \approx \exp\left\{-\mathrm{i}\int_{-\infty}^{t} \mathrm{d}t'\,E_0(n,t')\right\}|N\rangle \tag{14}$$

so that (10) gives

$$\gamma(n) \approx \gamma_0(n). \tag{15}$$

Systematic improvements can, however, be achieved by not neglecting the off-diagonal terms. Instead, $H_1(t)$ is regarded as a new hamiltonian with new eigenstates $|n_1(t)\rangle$ and new eigenvalues $E_1(n,t)$, and the transformation repeated, leading to a new representation $|\psi_2(t)\rangle$ and a further hamiltonian $H_2(t)$. Obviously the procedure can be iterated according to the scheme

$$\left.\begin{aligned} H_{k+1} &= U_k^\dagger H_k\,U_k - \mathrm{i}\,U_k^\dagger U_k, \\ \text{i.e.}\qquad \langle M\,|\,H_{k+1}|\,N\rangle &= E_k(n)\,\delta_{MN} - \frac{\mathrm{i}\,\langle M_k\,|\dot{H}_k|\,n_k\rangle}{E_k(n) - E_k(m)}(1-\delta_{MN}), \end{aligned}\right\} \tag{16}$$

where

$$U_k\,|N\rangle = |n_k\rangle, \quad H_k\,|n_k\rangle = E_k(n)\,|n_k\rangle, \quad \langle n_k\,|\,\dot{n}_k\rangle = 0. \tag{17}$$

(Iteration does not change the initial states $|N\rangle$, because of the assumed smoothness of H_0.)

At the kth iteration step,

$$\langle N|\psi_0(+\infty)\rangle = \langle N|U_0(+\infty)\,U_1(+\infty)\ldots U_k(+\infty)|\psi_{k+1}(+\infty)\rangle$$
$$= \exp\left\{\mathrm{i}\sum_{j=0}^{k}\gamma_j(n)\right\}\langle N|\psi_{k+1}(+\infty)\rangle, \tag{18}$$

where $\gamma_j(n)$ are the anholonomies of the cycled hamiltonians $H_j(t)$. We can stop at this iteration by neglecting the off-diagonal elements in H_{k+1}. This gives the *kth phase approximant*

$$\gamma(n) \approx \gamma^{(k)}(n) \equiv \sum_{j=0}^{k}\gamma_j(n) + \int_{-\infty}^{\infty} \mathrm{d}t\,[E_0(n,t) - E_k(n,t)]. \tag{19}$$

The sequence of approximants is not a perturbation series in the adiabatic parameter ϵ, because even $\gamma^{(1)}$ involves ϵ to infinitely high order (of course $\gamma^{(0)} = \gamma_0$ is independent of ϵ). Rather, the iterations can be regarded as successive superadiabatic transformations to moving frames (in Hilbert space) attempting to cling ever more closely to the evolving state $|\psi_0\rangle$ (we will see in §4 that the attempts ultimately fail).

It is instructive to digress and consider iteration schemes that are not based on the parallel-transport law (3). An obvious class of alternatives (infinitely many) is to require the $|n_k(t)\rangle$ to return exactly to $|N\rangle$ as $t \to +\infty$. This would eliminate the anholonomies of the U_k, but would change the diagonal elements of the iterated hamiltonians to

$$\langle N|H_{k+1}(t)|N\rangle = E_k(n) - \mathrm{i}\langle n_k|\dot{n}_k\rangle, \tag{20}$$

where E_k and $|n_k\rangle$ are of course different from those in the previous scheme. Instead of (19) we would have

$$\gamma(n) \approx \int_{-\infty}^{\infty} \mathrm{d}t\,[E_0(n,t) - E_k(n,t) - \mathrm{Im}\langle n_k|\dot{n}_k\rangle], \tag{21}$$

so that in this form of iteration the phase arises from the approximate eigenvalue of H_{k+1}, and so its derivation appears entirely 'dynamical', even for $k = 0$! (γ_0 itself is geometric, regardless of how it is derived, because it does not depend on ϵ). Obviously it is possible to construct intermediate iteration schemes, in which the derivation appears as partly anholonomic and partly dynamical. The precise classical analogue of this interpretational ambiguity can be seen in the contrasting treatments of adiabatic angles by Hannay (1985) (anholonomic) and Berry (1985) (dynamical). The reason for choosing the iteration scheme based on (3) is firstly that it is unique and secondly that the corrections to the hamiltonian at each stage (16) are entirely in the off-diagonal terms and thus higher order in ϵ.

3. Spin-$\frac{1}{2}$ systems

We take

$$H_0(t) = \boldsymbol{R}_0(t)\cdot\boldsymbol{\sigma}, \tag{22}$$

where $\boldsymbol{R}_0 \equiv (X_0\,Y_0, Z_0)$ and $\boldsymbol{\sigma}$ is the vector spin-$\frac{1}{2}$ operator. Thus

$$H_0 = \frac{1}{2}\begin{pmatrix} Z_0 & X_0 - \mathrm{i}\,Y_0 \\ X_0 + \mathrm{i}\,Y_0 & -Z_0 \end{pmatrix}. \tag{23}$$

The transformation (12) will generate a new hamiltonian $H_1(t) = \boldsymbol{R}_1(t)\cdot\boldsymbol{\sigma}$, and the aim of this section is to find the explicit form of this operator.

For simplicity of writing we temporarily omit the suffixes zero. Define unit vectors $\boldsymbol{r}(t)$, $\boldsymbol{v}(t)$, $\boldsymbol{w}(t)$, and positive scalars $R(t)$, $V(t)$, by

$$\boldsymbol{R} \equiv R\boldsymbol{r}, \quad \dot{\boldsymbol{r}} \equiv V\boldsymbol{v}, \quad \boldsymbol{w} \equiv \boldsymbol{r}\times\boldsymbol{v}, \tag{24}$$

and think of $\boldsymbol{r}$ as a radius vector of the unit sphere. Then the cycle of $H_0(t)$ is represented by transport of the triad $\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{w}$ round a circuit C_0 on the sphere (figure 1). The eigenvalues of H are $\pm\frac{1}{2}R(t)$, and the corresponding eigenstates $|n(t)\rangle$ will be denoted by $|\pm(t)\rangle$, or often simply by $|\pm\rangle$; these states depend on $\boldsymbol{r}(t)$ but not $R(t)$.

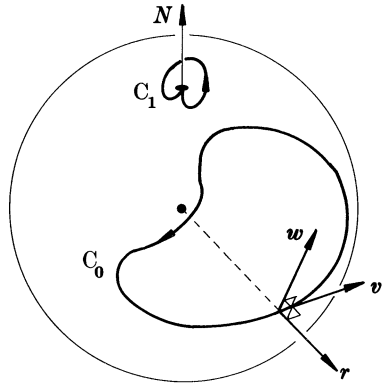

FIGURE 1. Transport of triad $\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{w}$ round initial circuit C_0 on the hamiltonian sphere, and iterated circuit C_1.

The operator $U(t)$ (6) turns the eigenstates $|\pm(-\infty)\rangle$ into the eigenstates $|\pm(t)\rangle$ by a sequence of infinitesimal rotations. It is shown in appendix A that the instantaneous angular velocity of the rotation is uniquely determined by (3), that is $\langle\pm|\dot{\pm}\rangle = 0$, to be the angular velocity $\boldsymbol{\Omega}_\parallel(t)$ of a frame *parallel-transported* with $\boldsymbol{r}$ over the spheres. This angular velocity is

$$\boldsymbol{\Omega}_\parallel = \boldsymbol{r}\times\dot{\boldsymbol{r}} = V\boldsymbol{w} \tag{25}$$

and must be distinguished from the different angular velocity $\boldsymbol{\Omega}_t$ of the triad $\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{w}$, which is

$$\boldsymbol{\Omega}_t = \boldsymbol{v}\times\dot{\boldsymbol{v}}. \tag{26}$$

Thus $U(t)$ is the time-ordered product

$$U(t) = T\exp\left\{-\mathrm{i}\int_{-\infty}^{t}\mathrm{d}t'\,\boldsymbol{\Omega}_\parallel(t')\cdot\boldsymbol{\sigma}\right\}. \tag{27}$$

To find the new operator H_1, we now use (12), which gives

$$H_1 = U^\dagger(\boldsymbol{R}-\boldsymbol{\Omega}_\parallel)\cdot\boldsymbol{\sigma}\,U. \tag{28}$$

This result has a purely classical origin (valid for any spin) in the transformation, to a non-inertial frame moving with $\boldsymbol{R}$ and rotating with angular velocity $\boldsymbol{\Omega}_\parallel$, of

the equation of motion for the expectation value $\langle\sigma\rangle$. (See, for example, Cina (1986), Suter *et al.* (1987), Anandan & Stodolsky (1987), and, for explicit calculations in terms of Hannay's angle, Berry (1986) and Gozzi & Thacker (1987)). From (13) and (28), the matrix representation in terms of the initial states is

$$H_1 = \begin{pmatrix} \frac{1}{2}R & \mathrm{i}V\langle +|\boldsymbol{\sigma}\cdot\boldsymbol{v}|-\rangle \\ -\mathrm{i}V\langle -|\boldsymbol{\sigma}\cdot\boldsymbol{v}|+\rangle & -\frac{1}{2}R \end{pmatrix}, \tag{29}$$

where use has been made of the fact that the off-diagonal elements of $\boldsymbol{\sigma}\cdot\boldsymbol{r}$ vanish.

To make this explicit we must evaluate $\langle +|\boldsymbol{\sigma}\cdot\boldsymbol{v}|-\rangle$. In Appendix A this is shown to be

$$\mathrm{i}\langle +|\boldsymbol{\sigma}\cdot\boldsymbol{v}|-\rangle = \tfrac{1}{2}\exp\left\{-\mathrm{i}\int_{-\infty}^{t}\mathrm{d}t'\Omega(t')\right\}, \tag{30}$$

where

$$\Omega \equiv (\boldsymbol{\Omega}_t - \boldsymbol{\Omega}_\parallel)\cdot\boldsymbol{r} = \boldsymbol{v}\times\dot{\boldsymbol{v}}\cdot\boldsymbol{r} = \boldsymbol{w}\cdot\dot{\boldsymbol{v}}. \tag{31}$$

Thus Ω measures the rate at which the $\boldsymbol{rvw}$ triad twists about $\boldsymbol{r}$, relative to the parallel-transported frame. The new hamiltonian (29) now becomes $H_1(t) = \boldsymbol{R}_1(t)\cdot\boldsymbol{\sigma}$ where (reinstating the suffixes)

$$Z_1 = R_0, \quad X_1 + \mathrm{i}Y_1 = V_0\exp\left\{\mathrm{i}\int_{-\infty}^{t}\mathrm{d}t'\Omega_0(t')\right\}, \tag{32}$$

As $\boldsymbol{r}_0(t)$ executes the loop C_0 representing H_0, the new unit vector executes a loop C_1 representing H_1 (figure 1). Because V_0 is adiabatically small (it is the speed at which $\boldsymbol{r}_0$ moves on the unit sphere), this new loop is very close to the north pole of the sphere. In fact C_1 resembles a cardioid with a cusp or corner at the pole, because $V_0 \to 0$ as $|t| \to \infty$. Iteration of the map from $\boldsymbol{R}_0$ to $\boldsymbol{R}_1$ gives $\boldsymbol{R}_2(t)$, $\boldsymbol{R}_3(t)\ldots$ and hence further loops $\mathrm{C}_2, \mathrm{C}_3, \ldots$. For small ϵ these loops rapidly diminish in size at first, and we might hope that they will continue to do so (especially because $R_{k+1} = (R_k^2 + V_k^2)^{\frac{1}{2}} > R_k$ so iteration takes H further from the degeneracy at $R = 0$). But this hope cannot be realized, as will be explained in §4.

To obtain the phase approximations $\gamma^{(k)}(\pm)$ from (19) we must determine the anholonomies $\gamma_j(\pm)$ from the unitary operators (27). These can be obtained by noting that the effect of all the infinitesimal rotations in the product (27) from $t = -\infty$ to $t = +\infty$ is a spinor rotation about the initial direction $\boldsymbol{r}(-\infty)$ (which of course is the same as the final direction) by the parallel transport angles A_j associated with the loops C_j. These are simply the *solid angles* subtended by the loops at the origin of the sphere, obtained from (31) as the total twist of the parallel frame about the $\boldsymbol{rvw}$ triad, plus the 2π rotation of that triad, namely

$$\begin{aligned} A_j &= 2\pi - \int_{-\infty}^{\infty}\mathrm{d}t\,\Omega_j(t) = 2\pi - \int_{-\infty}^{\infty}\mathrm{d}t\,\boldsymbol{v}\times\dot{\boldsymbol{v}}\cdot\boldsymbol{r} \\ &= 2\pi - \oint_{\mathrm{C}_j}\mathrm{d}\boldsymbol{r}\cdot\boldsymbol{r}''\times\boldsymbol{r}, \end{aligned} \tag{33}$$

where primes denote differentiation with respect to arc length on the sphere.

Thus with the z axis temporarily along $\boldsymbol{r}(\pm\infty)$ we have

$$U_j(+\infty) = \exp\left\{-\tfrac{1}{2}\mathrm{i}A_j\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right\} = 1\cos(\tfrac{1}{2}A_j) - \mathrm{i}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\sin(\tfrac{1}{2}A_j) \tag{34}$$

so that

$$U_j(+\infty)\begin{pmatrix}a\\ b\end{pmatrix} = \begin{pmatrix}\exp\{-\tfrac{1}{2}\mathrm{i}A_j\}a\\ \exp\{+\tfrac{1}{2}\mathrm{i}A_j\}b\end{pmatrix} \tag{35}$$

giving

$$\gamma_j(\pm) = \mp\tfrac{1}{2}A_j \tag{36}$$

as found by Berry (1984). The energies in (19) are simply $E_k(\pm) = \pm\frac{1}{2}R_k$, so the phase approximants are

$$\gamma^{(k)}(\pm) = \mp\frac{1}{2}\left\{\sum_{j=0}^{k} A_j + \int_{-\infty}^{\infty} \mathrm{d}t\,[R_k(t) - R_0(t)]\right\}. \tag{37}$$

As illustration, consider the lowest-order approximations to the phase when C_0 is a circle of latitude on the unit sphere, with polar angle θ and azimuth $\phi(t)$ satisfying $\phi(+\infty) - \phi(-\infty) = 2\pi$. Thus

$$\boldsymbol{R}_0 = \boldsymbol{r}_0 = (\sin\theta\cos\phi(t), \sin\theta\sin\phi(t), \cos\theta). \tag{38}$$

The speed (24) on the sphere is

$$V_0 = \sin\theta\dot{\phi} \tag{39}$$

and the twist (31) is

$$\Omega_0 = \cos\theta\dot{\phi} \tag{40}$$

so (32) gives the new loop C_1 as $\boldsymbol{r}_1(t) = \boldsymbol{R}_1(t)/R_1(t)$, where

$$\boldsymbol{R}_1(t) = (\sin\theta\dot{\phi}\cos\{\phi(t)\cos\theta\}, \sin\theta\dot{\phi}\sin\{\phi(t)\cos\theta\}, 1). \tag{41}$$

Now we introduce an adiabatic ϵ by

$$\phi(t) \equiv \Phi(\tau), \quad \tau \equiv \epsilon t. \tag{42}$$

Then it is not difficult to show that the anholonomies A_j in (37) are even in ϵ while the 'dynamical' integrals over R_k are odd. Apart from

$$A_0 = 2\pi(1 - \cos\theta), \tag{43}$$

which is of course independent of ϵ, all the other terms in (37) are of infinite order in ϵ. Thus

$$\int_{-\infty}^{\infty} \mathrm{d}t\,[R_1(t) - R_0(t)] = \frac{1}{\epsilon}\int_{-\infty}^{\infty} \mathrm{d}\tau\,[(1 + \epsilon^2\sin^2\theta\Phi'^2(\tau))^{\frac{1}{2}} - 1], \tag{44}$$

where the prime denotes $\mathrm{d}/\mathrm{d}\tau$. The first three terms of an expansion are contained in the first iteration $\gamma^{(1)}(\pm)$, and are

$$\gamma_{\pm}^{(1)}(\pm) \approx \mp\left\{\pi(1 - \cos\theta) + \tfrac{1}{4}\epsilon\sin^2\theta\int_{-\infty}^{\infty}\mathrm{d}\tau\,\Phi'^2(\tau) + \tfrac{1}{4}\epsilon^2\sin^2\theta\cos\theta\int_{-\infty}^{\infty}\mathrm{d}\tau\,\Phi'^3(\tau)\right\}. \tag{45}$$

The terms originate in A_0, R_1 and A_1 respectively. Garrison (1986) has obtained the first two terms of (45) by adiabatic perturbation (ϵ-expansion).

4. Inevitability of divergence

To get the kth phase approximant (19) we neglected the off-diagonal terms in H_{k+1} and so approximated $\langle N|\psi_{k+1}(+\infty)\rangle$ in (18) by a pure phase factor. This ignores transitions to other states, which will cause the survival probability $|\langle N|\psi_{k+1}(+\infty)\rangle|^2$ to deviate from unity. The transition probability is typically exponentially small (Hwang & Pechukas 1977), i.e.

$$\Delta(\epsilon) \equiv 1-|\langle N|\psi_k(+\infty)\rangle|^2 \sim \exp\{-1/\epsilon\}; \tag{46}$$

$\Delta(\epsilon)$ is independent of the order of iteration k (cf. (18)). The sequence $\gamma^{(k)}(n)$ cannot converge for finite ϵ because this would imply $\Delta = 0$. Therefore the sequence must diverge: the true phase must reflect the non-analyticity of the survival amplitude, unlike the terms in (19), which although of infinite order in ϵ are nevertheless analytic at $\epsilon = 0$.

We expect the terms $\gamma_j(n)$ to get smaller at first and then increase. This is the typical behaviour of an asymptotic expansion (Dingle 1973), and it is reasonable to hope that the best approximant is the one for which $|\gamma^{(k+1)}(n)-\gamma^{(k)}(n)|$ is smallest (excluding perversities such as oscillations in this quantity) and that this value is of the same order as the non-adiabaticity (see Balian *et al.* (1978) for a numerical demonstration of a related phenomenon).

We can illustrate the inevitable divergence with the loops C_j on the unit sphere (figure 1) which represents the successive hamiltonians $H_j(t)$ for a spin-$\frac{1}{2}$ particle. For small ϵ the first iterated loop C_1, and many subsequent ones, will be small and close to the north pole. If we write the radius vector as $\boldsymbol{r} = (x, y, z)$ then $z \approx 1$ and we can approximate the loops as lying in the tangent plane at the pole. Parallel transport is now ordinary euclidean parallel translation, and in the iteration (32) $\int_{-\infty}^{t} \mathrm{d}t'\boldsymbol{\Omega}(t')$ is the direction of the tangent to the loop at t, relative to that at $t = -\infty$. Denoting $x+\mathrm{i}y$ by ζ we find that (32) reduces to the simple iteration

$$\zeta_{j+1}(t) = \dot{\zeta}_j(t)/R_j(t). \tag{47}$$

When investigating the behaviour of the loops thus generated we can set $R_j(t) = 1$, because the successive radii differ little from $R_0(t)$ (cf. 31 which shows that $R_1^2 = R_0^2 + V_0^2$) and can be reduced to unity by the time rescaling $\mathrm{d}t \to R_0(t)\,\mathrm{d}t$. Thus (47) becomes the iterated hodograph transformation of mechanics, namely

$$\zeta_k(t) = \mathrm{d}^k\zeta_0(t)/\mathrm{d}t^{k+1}. \tag{48}$$

The loop C_k is generated in the xy plane by letting t run from $-\infty$ to $+\infty$. To describe adiabatic circuits we consider t to appear in the combination ϵt. Then ζ_k contains a factor ϵ^k and the C_k initially decrease in size. It would be reasonable to expect this decrease to continue, but it does not. The surprising fact is that, for almost all initial loops $\zeta_0(t)$, the C_k ultimately get bigger, and moreover for small ϵ the nature of the increase is *universal*. Furthermore, the winding number of C_k, defined as the number of rotations of the tangent as the loop is traversed, exceeds that of C_{k-1} by $\frac{1}{2}$ (alternate loops have cusps at $\zeta = 0$).

To justify these assertions we begin by recalling the assumption that $H_0(t)$, and

hence $\zeta_0(t)$, is smooth, and interpret this as analyticity in a strip about the t axis. Thus the Fourier transform $\bar{\zeta}_0(\omega)$, defined by

$$\zeta_0(t) = \int_{-\infty}^{\infty} d\omega\, \bar{\zeta}_0(\omega) \exp\{-i\omega\epsilon t\} \tag{49}$$

decays exponentially as $|\omega| \to \infty$, the exponents being the imaginary parts of the singularities of $\zeta_0(t)$ nearest to the real axis in the upper and lower halves of the ϵt plane. If these singularities are

$$\tau_+ = \tau_{1+} + i\tau_{2+}, \quad \tau_- = \tau_{1-} - i\tau_{2-} \quad (\tau_{2+}, \tau_{2-} > 0) \tag{50}$$

then
$$\bar{\zeta}_0(\omega) \to A_\pm \exp\{i\omega\tau_{1\pm}\} \exp\{-|\omega|\tau_{2\pm}\} \quad \text{as} \quad \omega \to \pm\infty. \tag{51}$$

The iterated loops (49) are given by (48) as

$$\zeta_k(t) = (-i)^k \int_{-\infty}^{\infty} d\omega\, (\epsilon\omega)^k \bar{\zeta}_0(\omega) \exp\{-i\omega\epsilon t\}. \tag{52}$$

For large k only the asymptotic form (51) of $\bar{\zeta}_0(\omega)$ contributes (because of the $(\epsilon\omega)^k$ factor) so that

$$\zeta_k(t) \to (-i\epsilon)^k k!\{A_+/[\tau_{2+} - i(\tau_{1+} - \epsilon t)]^{k+1} + (-1)^k A_-/[\tau_{2-} + i(\tau_{1-} - \epsilon t)]^{k+1}\}. \tag{53}$$

The term with the smaller of $\tau_{2\pm}$ dominates exponentially, so that after a trivial shift of time origin and redefinition of ϵ as $\epsilon/\min\{\tau_{2\pm}\}$ the kth loop takes the universal form

$$\zeta_k(t) \to \frac{A(i\epsilon)^k k!}{(1 - i\epsilon t)^{k+1}} = A[\epsilon^k k!/(1+\epsilon^2 t^2)^{\frac{1}{2}(k+1)}] \times \exp\{i[\tfrac{1}{2}k\pi + (k+1)\arctan \epsilon t]\} \quad \text{as} \quad k \to \infty. \tag{54}$$

These universal loops C_k are Maclaurin's sinusoidal spirals (Lawrence 1972), some of which are shown in figure 2. In polar coordinates defined by $r = i^k \exp\{i\phi\}$ their equation is

$$r_k(\phi) = A\epsilon^k k! \cos^{k+1}\{\phi/(k+1)\} \tag{55}$$

(C_0 is a circle, C_1 a cardioid and C_2 Cayley's sextic). The maximum radius (at $\phi = 0$) is $r_k = A\,\epsilon^k\, k!$. This decreases at first (because of ϵ^k) but ultimately increases (because of $k!$). The smallest maximum radius occurs when $k \approx \epsilon^{-1}$ and is

$$r_{1/\epsilon}(0) \approx A(2\pi/\epsilon)^{\frac{1}{2}} \exp\{-1/\epsilon\}. \tag{56}$$

The kth loop has winding number $\frac{1}{2}k + 1$; the initial and final windings ($t \approx \pm(k+1)/\pi\epsilon$) have radii smaller than the largest radius ($t = 0$) by a factor $[\pi/(k+1)]^{k+1}$.

The universality of the sinusoidal spirals can be described alternatively by saying that these curves are the attractors of the hodograph map in the space of loops. In view of the well-known instability of differentiation, the existence of attractors is remarkable, especially when considered backwards: the almost spirals C_k (k large), when iterated under the inverse map which is an integration and therefore supposedly stabilizing, must diversify into the infinite variety of

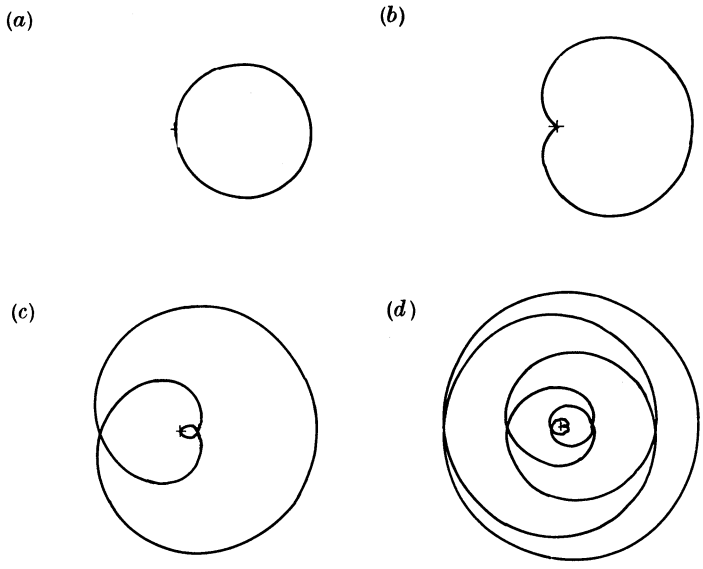

FIGURE 2. Universal loops (55) (sinusoidal spirals) for (*a*) $k = 0$; (*b*) $k = 1$; (*c*) $k = 9$; (*d*) $k = 50$. The loops are normalized to have the same maximum distance from the origin (which is reached at $t = \pm\infty$). The kth loop has $\frac{1}{2}k+1$ windings (not all visible in (*c*) and (*d*) because they are so small).

possible C_0. The resolution of the apparent paradox must lie in the assumed analyticity of C_0.

The asymptotic behaviour of the loops is reflected in the phase approximants $\gamma^{(k)}$. In the north-pole plane approximation (48) the solid angle A_k is just the euclidean area of C_k, namely

$$A_k = \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{Im}\, \zeta_k^* \dot{\zeta}_k \tag{57}$$

and the difference between successive radii is (cf. 32)

$$R_{k+1} - R_k = (R_k^2 + V_k^2)^{\frac{1}{2}} - R_k \approx \tfrac{1}{2}|\dot{\zeta}_k|^2 \tag{58}$$

because we have normalized R_k approximately to unity. Thus, roughly, the difference between successive approximants (37) is, with (48),

$$|\gamma^{(k+1)} - \gamma^{(k)}| \approx \frac{1}{4}\int_{-\infty}^{\infty} \mathrm{d}t\{\mathrm{Im}\,(\dot{\zeta}_k^*\, \ddot{\zeta}_k) + |\dot{\zeta}_k|^2\} \tag{59}$$

With the universal (54) this becomes

$$|\gamma^{(k+1)} - \gamma^{(k)}| \approx \tfrac{1}{4}A^2\,[(k+1)!]^2\, \epsilon^{2k+1}\,(\epsilon(k+\tfrac{3}{2})+1)\, I_{k+2}, \tag{60}$$

where $$I_k \equiv \int_{-\infty}^{\infty} \mathrm{d}\tau/(1+\tau^2)^k = 2\int_0^{\frac{1}{2}\pi} \mathrm{d}\theta\, \cos^{2(k-1)}\theta \to \left(\frac{\pi}{k}\right)^{\frac{1}{2}} \quad \text{as} \quad k \to \infty. \tag{61}$$

For small ϵ, (60) falls to a minimum when $k \approx \epsilon^{-1}$, whose value is of order $\exp\{-1/\epsilon\}$. When units are reinstated, the critical k acquires the following physical interpretation: ϵ^{-1} is the ratio of the average transition frequency between the two instantaneous eigenstates and the average rate of adiabatic change of

$\ln H_0(t)$. With this interpretation, $\exp\{-1/\epsilon\}$ is indeed the size of the nonadiabaticity (Hwang & Pechukas 1977).

It is possible to construct loops C_0 whose iterates do not fall into the universality class just discussed. One way is to make $\zeta_0(t)$ have its 'nearest singularity' actually *on* the real t axis whilst possessing all derivatives. For example, if $\zeta_0 \sim 1-\exp\{-1/\epsilon|t|\}$ the smallest loop occurs for iteration $k \sim \epsilon^{-\frac{1}{2}}$ and has radius of order $\exp\{\epsilon^{-\frac{1}{2}}\}$. The opposite situation is for $\zeta_0(t)$ to be so smooth that its 'nearest singularity' lies infinitely far from the axis. For example, if $\zeta_0 \sim \exp\{-(\epsilon t)^2\}$ the smallest loop occurs for iteration $k \sim \epsilon^{-2}$ and has radius of order $\exp\{\epsilon^{-2}\}$. Another possibility is for the imaginary parts $\tau_{2\pm}$ in (50) to be equal, so that neither of the two contrary loops in (53) dominates; one example is when $\zeta_0(t)$ is real, that is C_0 is simply a back-and-forth swinging enclosing no area (then there is no anholonomy and γ is purely dynamical). It does seem, however, that whatever the form of $\zeta_0(t)$ (provided all derivatives exist, and vanish as $|t| \to \infty$) the loops do eventually grow, but I have not been able to construct a general proof.

The nonadiabaticity, as expressed by the transition probability $\Delta(\epsilon)$ defined by (46), can be estimated by perturbation theory, using $|N\rangle$ as the unperturbed state. For spin-$\frac{1}{2}$ systems it is tempting to employ perturbation theory in the north pole plane approximation, applying it to the hamiltonian for the iteration for which C_k is smallest. However, this gives only a crude approximation, for reasons worth exploring because they illuminate a curious general feature of the adiabatic approximation.

Application of standard time-dependent perturbation theory to the iterated hamiltonian (13) gives the transition probability $\Delta(\epsilon)$ in (46) as the sum of the probabilities of transitions to states $M \neq N$:

$$\Delta(\epsilon) \approx \sum_{M \neq N} \left| \int_{-\infty}^{\infty} \mathrm{d}t \, \frac{\langle m_0 | \dot{H}_0 | n_0 \rangle}{E_0(n) - E_0(m)} \exp\left\{ \mathrm{i} \int_{-\infty}^{t} \mathrm{d}t' \, [E_0(m) - E_0(n)] \right\} \right|^2, \tag{62}$$

For a spin-$\frac{1}{2}$ system, starting (say) in $|+\rangle$, this gives, for the probability that at $t = +\infty$ there has been a transition to $|-\rangle$,

$$\Delta(\epsilon) \approx \frac{1}{4} \left| \int_{-\infty}^{\infty} \frac{V_0(t)}{R_0(t)} \exp\left\{ \mathrm{i} \int_{-\infty}^{t} \mathrm{d}t' \, [\Omega_0(t') - R_0(t')] \right\} \right|^2, \tag{63}$$

where use has been made of (29) and (30). Both the preceding formulae are independent of the order of iteration.

In the north-pole plane approximation with $R_0 = 1$, (63) becomes

$$\Delta(\epsilon) \approx \frac{1}{4} \left| \int_{-\infty}^{\infty} \mathrm{d}t \, \zeta_0(t) \exp\{-\mathrm{i}t\} \right|^2. \tag{64}$$

This too is independent of the order of iteration, as can be seen from (48) and integration by parts. Substituting the universal loop (54) gives

$$\left.\begin{aligned} \Delta(\epsilon) &\approx \frac{A^2}{4} \left| \int_{-\infty}^{\infty} \mathrm{d}t \, (1 - \mathrm{i}\epsilon t)^{-1} \exp\{-\mathrm{i}t\} \right|^2 \\ &= \frac{A^2 \pi^2}{\epsilon^2} \exp\{-2/\epsilon\} \quad \text{if} \quad \epsilon > 0 \\ &= 0 \quad \text{if} \quad \epsilon < 0. \end{aligned}\right\} \tag{65}$$

The two cases $\epsilon > 0$ and $\epsilon < 0$ correspond to opposite senses for the traversals of the loops and hence to an original hamiltonian $H_0(t)$ and its time reverse $H_0(-t)$. It is not surprising that time reversal can lead to very different transition probabilities because almost all the hamiltonians which give rise to anholonomy lack time-reversal symmetry. What *is* surprising – and this is the curious feature mentioned earlier – is that the phase is insensitive to this qualitative distinction to all orders of adiabatic iteration: the approximants (19) merely change sign under time reversal.

However, the extreme difference between $\epsilon > 0$ and $\epsilon < 0$ in (65) is an artefact of the north-pole plane approximation, arising from the fact that for $\epsilon < 0$ the perturbation $(1-\mathrm{i}\epsilon t)^{-1}$ has no negative-frequency components to stimulate the transition from $|+\rangle$ to $|-\rangle$. Without this approximation, but still taking C_0 as a circle, not necessarily small, as given by (38), the perturbation formula (63) gives, on making use of (39) and (40),

$$\Delta(\epsilon) \approx \frac{\sin^2\theta}{4}\left|\int_{-\infty}^{\infty} \mathrm{d}t\,\dot{\phi}(t)\exp\{\mathrm{i}[\phi(t)\cos\theta - t]\}\right|^2. \tag{66}$$

Now take

$$\phi(t) = 2\arctan\epsilon t, \tag{67}$$

which gives the same form of cycling as the universal loop (54). Then integration by parts gives

$$\Delta(\epsilon) \approx \frac{\tan^2\theta}{4\epsilon^2}\left|\int_{-\infty}^{\infty} \mathrm{d}\tau\left(\frac{1+\mathrm{i}\tau}{1-\mathrm{i}\tau}\right)^{\cos\theta}\exp\{-\mathrm{i}\tau/\epsilon\}\right|^2. \tag{68}$$

Changing the sign of ϵ has the same effect as changing θ to $\pi-\theta$, as it should because the effects on $|+\rangle$ of time reversal and latitude reversal of C_0 are the same.

In appendix B it is shown that the asymptotic form of (68) for small positive ϵ is

$$\Delta(\epsilon) \approx [\sin\pi\cos\theta)\tan\theta\Gamma(1-\cos\theta)2^{\cos\theta}]^2\exp\{-2/\epsilon\}/\epsilon^{2\cos\theta}. \tag{69}$$

Near the poles and the equator this has the limiting forms

$$\left.\begin{aligned}\Delta(\epsilon) &\to 4\pi^2\theta^2\exp\{-2/\epsilon\}/\epsilon^2 && \text{as}\quad \theta\to 0,\\ &\to \pi^2\exp\{-2/\epsilon\} && \text{as}\quad \theta\to\tfrac{1}{2}\pi,\\ &\to \tfrac{1}{16}\pi^2(\pi-\theta)^6\epsilon^2\exp\{-2/\epsilon\} && \text{as}\quad \theta\to\pi.\end{aligned}\right\} \tag{70}$$

The sense in which (65) is a crude approximation is now evident; instead of a discontinuity between $\epsilon > 0$ and $\epsilon < 0$ there is a smooth transition involving θ, which shows that time reversal does not make Δ vanish but reduces its value by ϵ^4.

5. Concluding remarks

The main result of this work is the formula (19) giving the phase approximants obtained from a (unique) succession of unitary transformations clinging ever closer to the evolving state. Successive approximants $\gamma^{(k)}(n)$ are correct to higher orders in the adiabatic parameter ϵ, but (19) is not a power series because each

approximant (except the lowest) contains ϵ to infinite order. Nevertheless, at all orders of iteration the scheme neglects non-adiabatic transitions, and because these are of order $\exp\{-1/\epsilon\}$ this quantity, rather than ϵ itself, can be regarded as the adiabatic parameter and then the entire sequence of approximants can be considered to be contained within the lowest-order adiabatic approximation (higher approximations to the exact phase (5) would involve powers of $\exp\{-1/\epsilon\}$).

For spin systems the unitary sequence can be interpreted geometrically as (initially) shrinking loops on the hamiltonian sphere. The loops could be observed, for example, by exploiting the fact that the expectation $\langle\boldsymbol{\sigma}\rangle$ evolves classically according to $\langle\dot{\boldsymbol{\sigma}}\rangle = \boldsymbol{R}_0 \times \langle\boldsymbol{\sigma}\rangle$. Then the unitary sequence corresponds to a sequence of transformations to rotating frames. Stopping at the kth such transformation, making the adiabatic approximation and transforming back to the original reference frame, we find that $\langle\boldsymbol{\sigma}\rangle$ follows not $\boldsymbol{R}_0(t)$ but $\boldsymbol{R}^{(k)}(t)$ which (cf. 28) includes corrections from the angular velocities $\boldsymbol{\Omega}_{\|}(t)$ of the successive frames, i.e.

$$\boldsymbol{R}^{(k)}(t) = \boldsymbol{R}_0(t) - \sum_{j=0}^{k-1} \boldsymbol{\Omega}_{\|j}(t). \tag{71}$$

Now, successive $\boldsymbol{\Omega}_{\|}$ are (initially) smaller (by ϵ), and generate loops C_k (§4) which in their own frames have increasing winding numbers. Therefore the motion of $\langle\boldsymbol{\sigma}\rangle$ is *a sequence of ever-finer nutations* forming a hierarchy reminiscent of Ptolemy's epicycles. Successive orders of iteration correspond to observing the motion with increasing resolution.

Several questions are raised by the divergence of the sequence of phase approximants. One concerns the universality of the shrinking-and-growing of the hamiltonian loops C_k for spin systems, when k is large, ϵ small and $H_0(t)$ analytic. This was derived within the north-pole plane approximation, and slight doubt lingers as to whether the result would survive inclusion of the effects of the curvature of the sphere. Assuming it does, another question is whether the divergence for non-spin systems has a similar adiabatic universality. (Of course for spins the universality we are discussing can last only for iteration numbers not much greater than $k \approx \epsilon^{-1}$; subsequent iterations will take the expanded loops C_k away from the north pole plane. What happens then? Is there an infinite sequence – possibly irregular – of further shrinking and growing when $k \gg \epsilon^{-1}$? Or do the windings continue to increase, leading to ultimate loops C_∞ covering the sphere densely?)

Finally, one wonders whether there are any systems for which the iteration would converge (or stop at some order) because the adiabatic approximation would be exact. This question is prompted by a spatial analogy: the existence of one-dimensional potentials $V(x)$ for which the semiclassical ('adiabatic') approximation is exact for some energies E, so that there is no reflection (i.e. no 'transition'). For example, with arbitrary real 'quantum momentum' $k_{\mathrm{qu}}(x)$ the local plane wave

$$\psi(x) = \exp\left\{\mathrm{i}\int_0^x \mathrm{d}x'\, k_{\mathrm{qu}}(x')\right\} \Big/ [k_{\mathrm{qu}}(x)]^{\frac{1}{2}} \tag{72}$$

is an exact solution of

$$\psi''(x)+k_{\rm cl}^2(x)\,\psi(x)=0 \tag{73}$$

provided it is related to the classical momentum $k_{\rm cl}=[(E-V)]^{\frac{1}{2}}$ by

$$k_{\rm qu}=[k_{\rm cl}^2+k_{\rm qu}^{\frac{1}{2}}(k_{\rm qu}^{-\frac{1}{2}})'']^{\frac{1}{2}}. \tag{74}$$

Then there is no coupling to the reflected wave which is the complex conjugate of (72). We can think of $k_{\rm qu}$ as the outcome of infinite order semiclassical iteration of (74), the lowest (W.K.B.) approximation being $k_{\rm qu}\approx k_{\rm cl}$. The analogue of γ is the phase of the transmitted wave (in this case entirely dynamical) referred to the W.K.B. phase, i.e.

$$\begin{aligned}\gamma&=\int_{-\infty}^{\infty}{\rm d}x\,(k_{\rm qu}-k_{\rm cl})\\&=\int_{-\infty}^{\infty}{\rm d}x\,k_{\rm qu}^{\frac{1}{2}}(k_{\rm qu}^{-\frac{1}{2}})''/\{k_{\rm qu}+[k_{\rm qu}^2-k_{\rm qu}^{\frac{1}{2}}(k_{\rm qu}^{-\frac{1}{2}})'']^{\frac{1}{2}}\},\end{aligned} \tag{75}$$

which from (74) is of infinite order in spatial slowness. The analogous adiabatic problem, of constructing a state $|\psi(t)\rangle$ evolving exactly as an eigenstate of some changing $H(t)$, seems much more difficult. Successive iterated hamiltonians would have to commute with each other. This is impossible for non-trivial spin systems, but it is conceivable that in other cases there would occur a conspiracy of the off-diagonal elements $\langle m_k|\dot{H}_k|n_k\rangle$ to allow at least one of the states to evolve adiabatically. (Of course I am not here denying the existence of the cyclic evolutions considered by Aharonov & Anandan 1987, because these involve states that return to themselves without having at every instant to be eigenstates of the driving hamiltonian; the spatial analogy is the Ramsauer–Townsend effect, in which perfect transmission is achieved without requiring $\psi(x)$ to be everywhere locally plane as in (72).)

Appendix A. Spin-$\frac{1}{2}$ calculations justifying (27) and (30)

The defining equation for $U(t)$ is (6), which can be written

$$U(t)\,|\pm(-\infty)\rangle=|\pm(t)\rangle. \tag{A 1}$$

Differentiating leads to

$$\dot{U}U^{\dagger}|\pm\rangle=|\dot{\pm}\rangle, \tag{A 2}$$

which on making use of $|+\rangle\langle+|+|-\rangle\langle-|=1$ becomes

$$\dot{U}=(|\dot{+}\rangle\langle+|+|\dot{-}\rangle\langle-|)\,U\equiv BU. \tag{A 3}$$

Then (27) follows if

$$B=-{\rm i}V\boldsymbol{w}\cdot\boldsymbol{\sigma}. \tag{A 4}$$

The diagonal elements $\langle \pm|B|\pm\rangle$ vanish because of orthogonality and $\langle \pm|\dot{\pm}\rangle = 0$. The diagonal elements $\langle \pm|\boldsymbol{w}\cdot\boldsymbol{\sigma}|\pm\rangle$ also vanish because $|\pm\rangle$ are eigenstates of $\boldsymbol{r}\cdot\boldsymbol{\sigma}$, and $\boldsymbol{w}$ is perpendicular to $\boldsymbol{r}$. The off-diagonal elements are

$$\langle \pm|B|\mp\rangle = \langle \pm|\dot{\mp}\rangle. \tag{A 5}$$

Differentiating the eigenequations

$$\boldsymbol{r}\cdot\boldsymbol{\sigma}|\pm\rangle = \pm\tfrac{1}{2}|\pm\rangle \tag{A 6}$$

gives

$$\langle \pm|\dot{\mp}\rangle = \mp V\langle \pm|\boldsymbol{v}\cdot\boldsymbol{\sigma}|\mp\rangle. \tag{A 7}$$

Now choose local axes in which $\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{w}$ lie along z, x, y respectively. Then

$$\langle +|\dot{-}\rangle = -\frac{V}{2}(1 \quad 0)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}0\\ 1\end{pmatrix} = -\frac{V}{2} \tag{A 8}$$

and

$$\langle +|B|\rangle = -\mathrm{i}V\langle +|\boldsymbol{w}\cdot\boldsymbol{\sigma}|-\rangle = -\mathrm{i}\frac{V}{2}(1 \quad 0)\begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix}\begin{pmatrix}0\\ 1\end{pmatrix} = \frac{-V}{2}. \tag{A 9}$$

Arguing similarly for $\langle -|\dot{+}\rangle$ we see that the operator equation (A 4) holds for all matrix elements and hence is true, thus implying (27).

To prove (30) we first show that $|\langle +|\boldsymbol{\sigma}\cdot\boldsymbol{v}|-\rangle| = \frac{1}{2}$:

$$\begin{aligned}\langle +|\boldsymbol{\sigma}\cdot\boldsymbol{v}|-\rangle\langle -|\boldsymbol{\sigma}\cdot\boldsymbol{v}|+\rangle &= \langle +|\boldsymbol{\sigma}\cdot\boldsymbol{v}(|-\rangle\langle -|+|+\rangle\langle +|)\boldsymbol{\sigma}\cdot\boldsymbol{v}|+\rangle\\ &= \langle +|(\boldsymbol{\sigma}\cdot\boldsymbol{v})^2|+\rangle = \tfrac{1}{4}.\end{aligned} \tag{A 10}$$

(The first equality is valid because $\langle +|\boldsymbol{\sigma}\cdot\boldsymbol{v}|+\rangle = 0$.) Thus we can write

$$\mathrm{i}\langle +|\boldsymbol{\sigma}\cdot\boldsymbol{v}|-\rangle = \tfrac{1}{2}\exp\{\mathrm{i}\mu(t)\} \tag{A 11}$$

To find an equation for μ, differentiate:

$$\tfrac{1}{2}\dot{\mu}\exp\{\mathrm{i}\mu\} = \langle \dot{+}|\boldsymbol{\sigma}\cdot\boldsymbol{v}|-\rangle + \langle +|\boldsymbol{\sigma}\cdot\dot{\boldsymbol{v}}|-\rangle + \langle +|\boldsymbol{\sigma}\cdot\boldsymbol{v}|\dot{-}\rangle. \tag{A 12}$$

The first and last terms vanish because

$$\langle \dot{\pm}|\boldsymbol{\sigma}\cdot\boldsymbol{v}|\mp\rangle = \langle \dot{\pm}|\pm\rangle\langle \pm|\boldsymbol{\sigma}\cdot\boldsymbol{v}|\mp\rangle + \langle \dot{\pm}|\mp\rangle\langle \mp|\boldsymbol{\sigma}\cdot\boldsymbol{v}|\mp\rangle = 0. \tag{A 13}$$

In the middle term, $\dot{\boldsymbol{v}}$ can be replaced by its component along $\boldsymbol{w}$, which from (31) gives, with (A 11)

$$\dot{\mu} = -\mathrm{i}\Omega\frac{\langle +|\boldsymbol{\sigma}\cdot\boldsymbol{w}|-\rangle}{\langle +|\boldsymbol{\sigma}\cdot\boldsymbol{v}|-\rangle}. \tag{A 14}$$

The matrix elements are just those previously evaluated in (A 7–A 9), so that

$$\dot{\mu} = -\Omega, \tag{A 15}$$

which with (A 10) and (A 11) gives (30).

Appendix B. Asymptotic evaluation of the integral (68)

Because of the exponent in (68), the integration contour can be deformed (for positive ϵ) into the negative half-plane to surround a cut extending from the branch point at $\tau = -\mathrm{i}$ to $\tau = -\mathrm{i}\infty$. On the right side we can take $\tau =$

$-\mathrm{i}+r\exp\{-\frac{1}{2}\mathrm{i}\pi\}$ (r from 0 to ∞) and on the left we can take $\tau=-\mathrm{i}+r\exp\{\frac{3}{2}\mathrm{i}\pi\}$ (r from ∞ to 0). Thus the integral becomes

$$-\mathrm{i}\exp\{-1/\epsilon\}\int_0^\infty \mathrm{d}r\,\frac{\exp\{-r/\epsilon\}(2+r)^{\cos\theta}}{r^{\cos\theta}}\left[\exp(\mathrm{i}\pi\cos\theta)-\exp(-\mathrm{i}\pi\cos\theta)\right]$$
$$=\frac{-\mathrm{i}\exp\{-1/\epsilon\}}{\epsilon^{(\cos\theta-1)}}\int_0^\infty \mathrm{d}x\,\frac{\exp\{-x\}(2+\epsilon x)^{\cos\theta}}{x^{\cos\theta}}\,2\mathrm{i}\sin(\pi\cos\theta).$$

For small ϵ the term ϵx can be neglected. The resulting integral is a Γ-function and squaring gives (69).

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