The Quantum Phase, Five Years After

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ABSTRACT

Classical parallel transport of vectors is described in a manner immediately generalizable to parallel transport of quantum states in parameter space. The associated anholonomy is the geometric phase. One realization of parallel transport is by adiabatic cycling of the parameters. The phase is the flux of a 2-form. The 2-form is equivalent to the antisymmetric part of a gauge-invariant quantum geometric tensor. The symmetric part of this tensor gives a natural metric on parameter space. If the parameters are themselves regarded as dynamical variables, their adiabatic dynamics are influenced by a gauge field depending on both parts of the tensor. Corrections to the geometric phase (of higher order in an adiabatic parameter) can be obtained by successive transformations to moving frames, thereby generating a renormalization map of circuits in the space of Hamiltonians; the iterates diverge in a universal way. This quantum renormalization is illustrated by classical Newtonian and Hamiltonian renormalizations for a pendulum with changing frequency. To conclude, there are some historical remarks about geometric phases.

1. Introduction

The kind invitation to write this survey article provides two welcome opportunities. First, to present the fundamentals of the subject in a new perspective, reflecting some of the many recent developments and including some new material; and second, to make some historical remarks, drawing attention to important early works and describing the genesis of my own ideas in this field.

Two concepts are crucial to the understanding of this dusty corner of quantum theory which the brooms of our understanding are beginning to disturb. They are anholonomy and adiabaticity.

Anholonomy is a geometrical phenomenon in which nonintegrability causes some variables to fail to return to their original values when others, which drive them, are altered round a cycle. The simplest anholonomy is in the parallel transport of vectors, two examples being the change in the direction of swing of a Foucault pendulum after one rotation of the earth, and the change in the direction of linear polarization of light along a twisting ray [1][2] or coiled optical fibre [3-6] whose direction is altered in a cycle. The anholonomy to be described here is quantum-mechanical, and concerns the phase of a state which is parallel-transported round a cycle [7]. Parallel transport of a quantum state will here be introduced as a simple generalization of parallel transport of a vector.

Adiabaticity is slow change and therefore denotes phenomena at the border between dynamics and statics. Adiabatic change provides the simplest (but not the only [8]) way to make quantum parallel transport happen. The variables which are cycled are parameters in the Hamiltonian of a system. If the cycling is slow, the adiabatic theorem [9] guarantees that the system returns to its original state. But it usually acquires a nontrivial phase, a manifestation of anholonomy, and this is the phenomenon of interest here.

2. Classical Parallel Transport

It is convenient to begin by obtaining the law for the ordinary parallel transport of a vector over the surface of a sphere, expressing it in a form enabling instantaneous generalization to quantum mechanics. Let the unit vector \mathbf{e} be transported by changing the unit radius vector \mathbf{r} (Fig.1) and making two demands: that $\mathbf{e} \cdot \mathbf{r}$ must remain zero and that the orthogonal triad (frame) containing \mathbf{e} and \mathbf{r} must not twist about \mathbf{r} , i.e., $\mathbf{\Omega} \cdot \mathbf{r} = 0$ where $\mathbf{\Omega}$ is the angular velocity of the triad. These conditions define parallel transport of \mathbf{e} and lead to the law

$$\dot{\mathbf{e}} = \mathbf{\Omega} \wedge \mathbf{e} \qquad \text{where} \qquad \mathbf{\Omega} = \mathbf{r} \wedge \dot{\mathbf{r}} \qquad (1)$$

This law is nonintegrable; when r returns to its original direction after a circuit C on the sphere, e does not return (in spite of never having been

twisted) but has turned through an angle $\alpha(C)$ which is the anholonomy now to be determined. Define $\mathbf{e}' \equiv \mathbf{r} \wedge \mathbf{e}$ (so that \mathbf{r} , \mathbf{e} , \mathbf{e}' form an orthogonal triad) and the complex unit vector

$$\psi \equiv (\mathbf{e} + i\mathbf{e}')/\sqrt{2} \tag{2}$$

in the plane perpendicular to r. In terms of ψ , the parallel transport law (1) (which holds for e' as well as e) takes the simple form

$$\operatorname{Im} \psi^* \cdot \dot{\psi} = 0 \qquad i.e., \qquad \operatorname{Im} \psi^* \cdot d\psi = 0 \qquad (3)$$

where $d\psi$ is the change in ψ resulting from a change $d\mathbf{r}$.

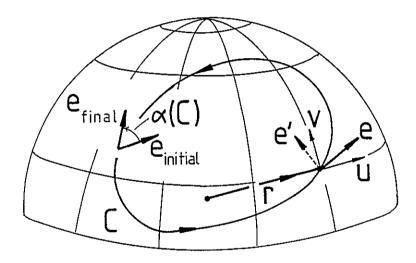


Figure 1. Rotation by $\alpha(C)$ after parallel transport of vector e round circuit C on a sphere.

To find $\alpha(C)$ we chart the passage of **e** and **e'** relative to a local basis of unit vectors $\mathbf{u}(\mathbf{r}), \mathbf{v}(\mathbf{r})$ (Fig.1) defined at each point on the sphere: For example, we could choose **u** and **v** to lie along the parallel of latitude θ and meridian of longitude ϕ at $\mathbf{r} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, i.e.,

$$\mathbf{u} = (-\sin\phi, \cos\phi, 0), \quad \mathbf{v} = (-\cos\theta\cos\phi, -\cos\theta\sin\phi, \sin\theta).$$
 (4)

Specifying a local basis is equivalent to specifying the complex unit vector

$$\mathbf{n}(\mathbf{r}) \equiv (\mathbf{u}(\mathbf{r}) + i\mathbf{v}(\mathbf{r}))/\sqrt{2}$$
 (5)

If the angle between the transported e and the local u is $\alpha(t)$, (2) and (5) give

 $\psi = \mathbf{n} \exp(-i\alpha) \tag{6}$

whence (3) gives the anholonomy as

$$\alpha(C) = \oint d\alpha = \operatorname{Im} \oint \mathbf{n}^* \wedge \cdot d\mathbf{n}$$

$$= \operatorname{Im} \iint_{\partial S = C} d\mathbf{n}^* \cdot d\mathbf{n}$$
(7)

where in the last equality Stokes' theorem has been used and the integral is over the area on the sphere bounded by C. It is an important result that the integrand in (7) is independent of the choice of local basis u, v: a change in this choice can be represented by a rotation $\mu(\mathbf{r})$ which induces the gauge transformation

$$\mathbf{n}(\mathbf{r}) \to \mathbf{n}'(\mathbf{r}) \exp \{i\mu(\mathbf{r})\}$$
 (8)

under which $d\mathbf{n}^* \wedge \cdot d\mathbf{n}$ is invariant.

In terms of arbitrary parameters X_1 , X_2 specifying r (i.e., position on the sphere), Eq. (7) can be written explicitly as

$$\alpha(C) = \operatorname{Im} \iint_{\partial S = C} dX_1 dX_2 \left(\partial_1 \mathbf{n}^* \cdot \partial_2 \mathbf{n} - \partial_2 \mathbf{n}^* \cdot \partial_1 \mathbf{n} \right)$$
(9)

where ∂_j denotes $\partial/\partial X_j$. The choice $X_1 = \theta$, $X_2 = \phi$, together with (4), yields the integrand $d\theta d\phi \sin\theta$, which is simply the area element on the sphere, leading to the old result that the anholonomy $\alpha(C)$ is the solid angle subtended by C at the centre of the sphere.

3. Quantum Parallel Transport

To make the generalization to quantum mechanics, we replace the complex unit vector ψ by a normalized quantum state $|\psi\rangle$, i.e., a unit vector in a Hilbert space, and position $\mathbf{r}=(X_1,X_2)$ on the sphere by position $X=(X_1,X_2,\ldots)$ in a space of parameters governing the physical system represented by $|\psi\rangle$. At each $X,|\psi\rangle$ is defined up to a phase (just as \mathbf{e} was defined up to a rotation at each \mathbf{r}). Then a natural transport law [10] governing the phase of $|\psi\rangle$ as X varies is provided by reinterpreting (3) as the connection

$$\operatorname{Im} \langle \psi | d\psi \rangle = 0. \tag{10}$$

Like (3), this law is nonintegrable: when X is taken round a circuit C, $|\psi\rangle$ returns with a changed phase. This change is the quantum geometric phase $\gamma(C)$; thus

$$\langle \psi_{\text{initial}} | \psi_{\text{final}} \rangle = \exp\{i\gamma(C)\}.$$
 (11)

To find γ we again introduce a local basis by choosing at each X a definite (and so of course single-valued) state $|n(X)\rangle$, relative to which $|\psi\rangle$ is defined by

$$|\psi\rangle = |n(X)\rangle \exp(i\gamma) \tag{12}$$

Then (10) gives

$$\gamma(C) = \oint d\gamma = -\operatorname{Im} \oint \langle n|dn\rangle$$

$$= -\operatorname{Im} \iint_{\partial S = C} \langle dn| \wedge |dn\rangle \equiv -\iint_{\partial S = C} V(X). \tag{13}$$

The integrand $V = \text{Im} (dn \wedge dn)$ is the phase 2-form, whose flux through C gives the geometric phase. V is invariant under the gauge transformation

$$|n(X)\rangle \to |n'(X)\rangle \equiv |n(X)\rangle \exp\{i\mu(X)\}$$
 (14)

For this mathematics to represent physics, it must be possible to implement the connection (10) by the Schrodinger equation

$$i\hbar|\dot{\Psi}\rangle = \hat{H}|\Psi\rangle$$
 (15)

governing the evolution of any state $|\Psi\rangle$. A simple way [7] is to incorporate the parameters X into the Hamiltonian and change them slowly. Then the adiabatic theorem guarantees that in the absence of degeneracies (a restriction that can be removed [46]) $|\Psi\rangle$ will cling to one of the eigenstates of $\hat{H}(X(t))$, defined by

$$\hat{H}(X)|\psi\rangle = E_n(X)|\psi\rangle \tag{16}$$

The adiabatic ansatz

$$|\Psi\rangle \approx |\psi\rangle \exp\left\{-\frac{i}{\hbar} \int_0^t dt' \, E_n(X(t'))\right\}$$
 (17)

then gives the connection (10) immediately upon projecting (15) onto $|\psi\rangle$. The state $|n(X)\rangle$ in the 2-form (13) is any solution of (16) with a definite phase at each X.

Because of (17), the total phase change of $|\Psi\rangle$ includes a dynamical part as well as the $\gamma(C)$ being studied here. Thus

$$\langle \Psi_{\text{final}} | \Psi_{\text{initial}} \rangle = \exp\{i(\gamma_d + \gamma C)\}$$
 (18)

where, for a circuit that takes a time T,

$$\gamma_d = -\frac{1}{\hbar} \int_0^T dt \ E_n(X(t)) \tag{19}$$

One might say that γ_d and $\gamma(C)$ give the system's best answers to two questions about its adiabatic circuit. For γ_d the question is: how long did your journey take? For $\gamma(C)$ it is: where did you go?

Aharanov and Anandan [8] give a different interpretation of parallel transport. They regard the parameters X as labelling the state, rather than \hat{H} , so that X_1, X_2, \ldots are coordinates in the projective Hilbert space that includes all quantum states, but where states differing only in phase (or normalization) are represented by the same point. Then a state $|\Psi\rangle$ evolving under Eq. (15) (not necessarily adiabatically) so as to return in T to the same X acquires a phase (18), with geometric part (13) (where the phase of $|n(X)\rangle$ is an arbitrary function of X) and dynamical part given by

$$\gamma_d = -\frac{1}{\hbar} \int_0^T dt \, \langle \Psi | \hat{H} | \Psi \rangle \tag{20}$$

instead of Eq. (19). The relation between the two approaches is that in the adiabatic case X parameterizes that part of the projective Hilbert space corresponding to the nth eigenstate of the chosen family of Hamiltonians $\hat{H}(X)$.

Several experiments have measured the geometric phase for particles, with spin 1/2 (neutrons [11]), spin 1 (photons [3]) and spin 3/2 (chlorine nuclei [12]). These depend on the result [7] that when \hat{H} is a rotationally symmetric function of the spin, *i.e.*,

$$\hat{H} = F(\boldsymbol{\sigma} \cdot \mathbf{X}) \tag{21}$$

where $\mathbf{X} = (X_1, X_2, X_3)$ and $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the vector spin operator, the geometric phase for the state with spin component n along \mathbf{X} is

$$\gamma_n(C) = -n\,\Omega(C) \tag{22}$$

where $\Omega(C)$ is the solid angle subtended by C at $\mathbf{X} = 0$.

These experiments all employ a superposition of eigenstates, rather than a single one, so that

$$|\Psi_{\text{initial}}\rangle = \sum_{n} a_{n} |n\rangle$$

$$|\Psi_{\text{final}}\rangle = \sum_{n} a_{n} |n\rangle \exp\{i(\gamma_{dn} + \gamma_{n}(C))\}$$
(23)

At the end, that is after X has been cycled, an observable \hat{A} , which does not commute with the final \hat{H} , is measured (for example with a polarizer). Thus

$$\begin{split} \langle \hat{A} \rangle &= \sum_{n} |a_{n}|^{2} \langle n | \hat{A} | n \rangle + 2 \operatorname{Re} \sum_{m \neq n} a_{n}^{*} a_{m} \langle m | \hat{A} | n \rangle \\ &\times \cos \left\{ \left[\gamma_{dn} + \gamma_{n}(C) \right] - \left[\gamma_{dm} + \gamma_{m}(C) \right] \right\}. \end{split}$$
 (24)

The oscillatory terms reveal $\gamma_n(C)$. This scheme has proved more convenient than the earlier suggestion [7] of splitting an ensemble of systems (e.g., a beam of particles) into two subensembles, one being driven by an \hat{H} which is cycled and the other by an \hat{H} which is not, and then recombining the subensembles to detect $\gamma(C)$ by interference. (That is, instead of using one state and two Hamiltonians it is preferable to use two states — at least — and one Hamiltonian.)

Hannay [13] found an analogue of the geometric phase for classical systems. This was based on the simple observation that a quantum system in an eigenstate is an oscillator (because of the time factor $\exp(-iE_nt/\hbar)$, so that classical oscillators should exhibit similar anholonomy when parameters that govern them are cycled. The phase is now an angle, which may be an angle in space, like that of a wheel, or — more commonly — an abstract angle variable in phase space as with a harmonic oscillator. If the classical system is multiply periodic (integrable) for all X, with N freedoms (that is, coordinates $q = (q_1 \cdots q_N)$ and momenta $p = (p_1 \cdots p_N)$ and Hamiltonian $H(\mathbf{q}, \mathbf{p}; X)$, its orbit for fixed X winds round an N-torus [14] in phase space, with N angle variables $\theta = (\theta_1 \cdots \theta_N)$ increasing uniformly. Conjugate to θ are N adiabatically conserved actions $\mathbf{I} = (I_1 \cdots I_N)$ which label the torus. After a slow cycle of X the angles have acquired shifts which contain a geometric as well as a dynamical part. For a spinning particle [15-17] this classical anholonomy is the angle shift given by ordinary parallel transport of a vector.

Underlying Hannay's angles is a *classical 2-form*. This is the classical limit of the phase 2-form in Eq. (13), and semiclassical asymptotics [18] provides the expression

$$V(X) \xrightarrow[\hbar \to 0]{} - \langle d\mathbf{p} \wedge \cdot d\mathbf{q} \rangle / \hbar \tag{25}$$

whose symbols should be interpreted as follows. The wedge product \wedge links the d's in parameter space. The scalar product \cdot links \mathbf{p} and \mathbf{q} . () denotes an average over the angles on the torus labelled \mathbf{I} which at X corresponds [19] to the quantum state $|n\rangle$, i.e., () = $\int_0^{2\pi} d\theta_1 \cdots d\theta_N / (2\pi)^N$. $d\mathbf{q}$ is the coordinate displacement linking corresponding points (labelled by the same θ) on the tori \mathbf{I} at X and X + dX, and similarly for $d\mathbf{p}$.

It is amusing to note that if the 2N variables q and p are replaced by the N complex variables

$$\mathbf{n} = (n_1 \cdots n_N) \equiv (\mathbf{q} + i\mathbf{p})/\sqrt{2\hbar}$$
 (26)

then (25) takes the form

$$V(X) \xrightarrow{p_{n-0}} \operatorname{Im} \langle d\mathbf{n}^* \wedge \cdot d\mathbf{n} \rangle \tag{27}$$

which bears a close formal resemblance both to the quantum expression (13) and the geometrical formula (7).

If the classical motion is not multiply periodic, that is if it is wholly or partly chaotic, the question of the classical limit of V is more delicate. It is tempting to claim that the limit is (25) for nonintegrable as well as integrable motion, but it is difficult to interpret the average $\langle \ \rangle$ and the displacements $d\mathbf{q}$ and $d\mathbf{p}$. In one of several interpretations, obtained by a semiclassical argument (not yet published) in collaboration with M. Wilkinson, $\langle \ \rangle$ denotes a time average over all points on an infinite orbit, and $d\mathbf{q}$ and $d\mathbf{p}$ link simultaneous points on the orbits for X and X+dX. For nonintegrable systems, however, it is not easy to express this result by replacing $\langle \ \rangle$ by a phase-space integral over the manifold explored by the orbit, because it is not clear what are then the 'corresponding points', linked by $d\mathbf{q}$ and $d\mathbf{p}$, on the manifolds for X and X+dX (for an ergodic system these are the two constant-energy surfaces).

4. The Quantum Geometric Tensor

The central mathematical object underlying the quantum phase is the 2-form $V = \operatorname{Im} \langle dn \wedge dn \rangle$. This is equivalent to an antisymmetric second-rank tensor field $V_{ij}(X)$ on the parameter space (or projective Hilbert space) with a quantum state $|n(X)\rangle$ defined at each point, namely

$$V_{ij}(X) = \operatorname{Im}\{\langle \partial_i n | \partial_j n \rangle - \langle \partial_j n | \partial_i n \rangle\}$$
 (28)

This tensor is invariant under the gauge transformation (14), but it is not the only such invariant tensor. More general is the quantum geometric tensor

$$T_{ij}(X) \equiv \langle \partial_i n | (1 - |n\rangle\langle n|) | \partial_j n \rangle \tag{29}$$

which is Hermitian, i.e., $T_{ij} = T_{ji}^*$. The projector $|n\rangle\langle n|$ is essential to the gauge invariance. The imaginary part of T_{ij} is simply $V_{ij}/2$, so we can write

$$T_{ij} = g_{ij} + iV_{ij}/2 \tag{30}$$

where g_{ij} is the real symmetric tensor field Re T_{ij} .

We know the quantum meaning of V_{ij} : its flux gives the phase $\gamma(C)$. Therefore, it is natural to ask whether g_{ij} has significance. The answer is that g_{ij} provides a natural means of measuring distances along paths in parameter space; it is the quantum metric tensor. To understand why, observe that a natural measure of the squared distance between two nearby quantum states is the deviation from unity of their scalar product. If the states are $|1\rangle$ and $|2\rangle$ this gives, for the distance between the corresponding points X_1 and X_2 in parameter space,

$$\Delta s_{12}^2 = 1 - |\langle 1|2\rangle|^2 \tag{31}$$

Taking the limit $1 \to 2$, and using the fact that all states are normalized, we obtain (using the summation convention for repeated indices i and j)

$$ds^{2} = \langle dn | (1 - |n\rangle\langle n|) | dn\rangle = \langle \partial_{i}n | (1 - |n\rangle\langle n|) | \partial_{j}n\rangle dX_{i}dX_{j}$$

= $T_{ij} dX_{i}dX_{j} = g_{ij} dX_{i}dX_{j}$ (32)

as claimed. The quantum tensor was introduced in an interesting paper by Provost and Vallee [50].

From its structure, g_{ij} can never give a negative ds^2 : in fact it is a positive semidefinite metric. Along a finite path (not necessarily closed) between $|1\rangle$ and $|2\rangle$, the quantum distance is

$$s_{12}(C) = \int_{1}^{2} (g_{ij} dX_{i} dX_{j})^{1/2}.$$
 (33)

Page [33] and Bouchiat and Gibbons [41] give explicit forms for some metrics on the full Hilbert and projective Hilbert spaces.

The simplest example is a 2-state system, for which \hat{H} has the form (21), with $\hat{\sigma}$ the 3 Pauli matrices. If we take X as a unit vector, specified by parameters θ , ϕ (polar angles), the eigenstates are

$$|+\rangle = \begin{pmatrix} \cos(\theta/2) e^{i\phi/2} \\ \sin(\theta/2) e^{-i\phi/2} \end{pmatrix}, \quad |-\rangle = \begin{pmatrix} \sin(\theta/2) e^{i\phi/2} \\ -\cos(\theta/2) e^{-i\phi/2} \end{pmatrix}$$
 (34)

For both of these, (32) gives $ds^2 = d\theta^2 + \sin\theta d\phi^2$, and this is the natural metric on the sphere of parameters (which in this case is also the projective Hilbert space).

Some interesting questions are suggested by this identification of g_{ij} as a metric on parameter space:

- (i) Do the geodesics, and in particular the shortest paths, connecting non-neighbouring states |1⟩ and |2⟩ have physical significance? One possibility, suggested by the work of Pancharatnam [20][21], is that the geodesics are the special paths along which the state preserves its phase in the sense that ⟨1|2⟩ is real. This is true for the 2-state system just discussed, but seems to fail otherwise (probably for reasons of codimension). It is worth remarking that as 2 → 1 the overlap ⟨1|2⟩ is real to second as well as first order in dX, for any path whatever.
- (ii) Can the geodesics be chaotic? This would require parameters X and states $|n(X)\rangle$ for which the Riemann curvature defined in terms of g_{ij} is negative (at least in some places) and the space is compact.
- (iii) Do families of geodesics (for example those issuing in different directions from the same point) exhibit the generic caustic singularities classified by catastrophe theory [22][23]? Do any such caustics have physical meaning? In 2-state systems the geodesics from X focus nongenerically at the

- antipodal point on the sphere, where the state is orthogonal to $|n(X)\rangle$, but again this appears to be a special situation.
- (iv) Is there any meaning or interest in quantizing the geodesic motion in parameter space, for example by taking as Hamiltonian the Laplace-Beltrami operator $g^{-1/2}\partial_i g^{-1/2}g_{ij}\partial_j$ (where $g \equiv \det g_{ij}$)? Such quantizations are different from that described in the next section.

5. Dynamics of the Parameters

Until now we have regarded X as classical parameters which can be altered arbitrarily and which are unaffected by the quantum system they drive. But no physical action is unilateral and in reality X are themselves dynamical variables of a 'heavy' system coupled to the 'light' system (what we have so far called 'the' system) and therefore subject to reaction from it. Indeed the earliest application of the adiabatic theorem was the Born-Oppenheimer theory of molecules, in which X are coordinates describing the positions of the (heavy) nuclei and the light system is the electrons. Recently it has been pointed out [24-27] that in lowest order the reaction of the light system on the heavy dynamics is through a gauge field consisting of a vector potential whose curl is the phase 2-form V, and a scalar potential. Here I will show that what the gauge field really depends on is the quantum geometric tensor T_{ij} of section 3.

Let the heavy momenta, conjugate to X_i , be P_i . Then a fairly general nonrelativistic quantum Hamiltonian for the coupled system is

$$\hat{H}_{\text{tot}} = \frac{1}{2} \sum_{ij} Q_{ij} \hat{P}_i \hat{P}_j + H(\hat{\xi}; \hat{X}),$$
 (35)

in which Q_{ij} is an inverse mass tensor, $\hat{\xi}$ are the dynamical variables of the light system (coordinates, momenta, spins, . . .) and H our previous Hamiltonian in which the X were regarded as parameters and which has eigenstates $|n(X)\rangle$ and energies $E_n(X)$. In the position representation for the heavy system, that is $\hat{P}_i = -i\hbar\partial_i$, the adiabatic ansatz is to write the full quantum state in the separated form

$$\langle X|\Psi\rangle \approx \Psi_{\text{heavy}}(X)|n(X)\rangle$$
 (36)

and to consider the effective Hamiltonian governing Ψ_{heavy} to be

$$\hat{H}_{\text{eff}} = \langle n(X) | \hat{H}_{\text{tot}} | n(X) \rangle. \tag{37}$$

In \hat{H}_{eff} the reaction of the light on the heavy system comes from the action of the gradient operators \hat{P}_i on the X-dependence of $|n\rangle$. A straightforward calculation gives

$$\hat{H}_{\text{eff}} = \frac{1}{2} \sum_{ij} Q_{ij} \left\{ \hat{P}_i - A_i(\hat{X}) \right\} \left\{ \hat{P}_j - A_j(\hat{X}) \right\} + \Phi(\hat{X}) + E_n(\hat{X})$$
 (38)

where

$$A_i(X) = i\hbar \langle n | \partial_i n \rangle \tag{39}$$

and

$$\Phi(X) = \frac{\hbar^2}{2} \sum_{ij} Q_{ij} g_{ij}(X)$$
 (40)

Here the emphasis is on the gauge potentials Φ and A_i — the scalar $E_n(X)$ is the 'potential surface' studied in conventional Born-Oppenheimer theory. Although (38) is a quantum Hamiltonian it can be used in suitable circumstances to calculate the *classical* motion of the heavy system, which will be affected by the fields A_i and Φ .

The physical effects of the vector potential A_i depend only on the 'magnetic' field

$$F_{ij} = \partial_i A_j - \partial_j A_i = -\hbar V_{ij} \tag{41}$$

(including its singularities and values in inaccessible regions — I am not denying the Aharonov-Bohm effect for heavy systems!). Thus the 'magnetic' field seen by the heavy system is the antisymmetric part of the quantum geometric tensor. The symmetric part of T_{ij} determines the 'electric' potential via Eq. (40). For an isotropic mass tensor, i.e., $Q_{ij} = \delta_{ij}/M$, Φ depends on $Tr\ g_{ij}$. It is a curious asymmetry that the 'electric' field depends on the gradients of g_{ij} whereas the 'magnetic' field depends on V_{ij} itself.

The singularities of the gauge field are the degeneracies X^* of the spectrum, where $E_n(X^*) = E_{n\pm 1}(X^*)$. It is already known [7] that the 'magnetic' field V_{ij} (2-form) has monopole singularities. From the definition (29) of T_{ij} it is clear that g_{ij} has similar singularities, so that the 'electric' field near X^* is an inverse-cube force.

The situation near a degeneracy can be described by a special case of a simple model, which is of independent interest (and which has been studied from a different viewpoint by Anandan and Aharonov [28]), where the spin s of one (light) particle is coupled to the spatial coordinates of a second otherwise free (heavy) particle. Thus

$$\hat{H}_{tot} = \frac{1}{2M}\hat{P}^2 + F(\hat{\mathbf{X}} \cdot \hat{\boldsymbol{\sigma}}) \tag{42}$$

Near a degeneracy the appropriate model is a 2-state light system, so that we should take $s = \frac{1}{2}$, with linear coupling $F \propto \mathbf{X} \cdot \boldsymbol{\sigma}$.

The eigenvalues of $\mathbf{X} \cdot \hat{\boldsymbol{\sigma}}$ are nX, where $X \equiv |\mathbf{X}|$ and $-s \leq n \leq s$. The quantum tensor for the state $|n\rangle$ can be shown to be

$$T_{ij}^{n}(X) = \frac{1}{2X^{2}} \left\{ \left(s(s+1) - n^{2} \right) \left(\mathbf{e_{i} \cdot e_{j}} - (\mathbf{e_{i} \cdot x})(\mathbf{e_{j} \cdot x}) \right) \mp in(\mathbf{e_{i} \wedge e_{j}}) \cdot \mathbf{x} \right\}$$

$$(43)$$

where $\mathbf{x} = \mathbf{X}/|\mathbf{X}|$ and $\mathbf{e_i}$ is the unit vector along the *i* direction. The metric tensor g_{ij} has a zero eigenvalue, corresponding to radial parameter

displacements, which simply scale H leaving the states $|n\rangle$ unaffected: radial motions cover zero distance.

From Eqs. (38)-(40), the classical Newtonian equation for the heavy particle involves the Lorentz force from the magnetic monopole and the 'electric' force

$$-\nabla_{\mathbf{X}}\Phi(\mathbf{X}) = -\frac{\hbar^2}{2M}\nabla_{\mathbf{X}}\operatorname{Tr} g_{ij} = \frac{\hbar^2(s(s+1)-n^2)}{MX^3}\mathbf{x}$$
(44)

This is of centrifugal type, and repels the parameters from a degeneracy (becoming significant at a distance of order $M^{-1/3}$), thereby tending to preserve the validity of the adiabatic approximation. We obtain, when the light particle is in the nth spin state,

$$M\ddot{\mathbf{X}} = \frac{S_z}{2X^3}\dot{\mathbf{X}}\wedge\mathbf{X} + \frac{\left(S^2 - S_z^2\right)}{MX^4}\mathbf{X} - \frac{nF'(nX)}{X}\mathbf{X}$$
 (45)

where $S_z \equiv n\hbar$ and $S^2 \equiv \hbar^2 s(s+1)$. This describes integrable motion, with conserved energy and modified angular momentum $M \mathbf{X} \wedge \dot{\mathbf{X}} - S_z \mathbf{X}/X$.

6. Adiabatic Renormalization

Now we return to the adiabatic scenario of section 3 and realize that γ_d and $\gamma(C)$ in Eq. (18) are but the first two terms in an infinite series involving powers of an adiabatic slowness parameter ϵ , influencing the dynamics through \hat{H} whose time-dependence enters in the combination ϵt . The dominant term is γ_d (Eq. 19) and is of order ϵ^{-1} . The next term is $\gamma(C)$, whose unique feature — and the reason for its being called geometric — is that it is independent of ϵ , and so depends only on the sequence of Hamiltonians along the circuit and not on its time history.

This uniqueness is not threatened by the observation that transformation to a moving frame (a common practice in problems involving spin [11]) can make $\gamma(C)$ appear 'dynamical' by making it emerge from a correction to the energy rather than as anholonomy: the geometric structure of $\gamma(C)$ is independent of how it is derived.

Transformations to moving frames have however another interest, in that they form the basis of a renormalization (iteration) technique for generating higher-order corrections to the phase. Details of the technique have been published elsewhere [29]; here I will outline the central idea, and give an example.

Let the Hamiltonian $\hat{H}_0(t)$ generating the quantum motion be cyclic, in the sense that $\hat{H}_0(+\infty) = \hat{H}_0(-\infty)$, and let it have instantaneous eigenstates $|n_0(t)\rangle$ and energies $E_0(n,t)$. The evolving state $|\Psi_0(t)\rangle$ is determined by

$$i|\dot{\Psi}_0(t)\rangle = \hat{H}_0(t)|\Psi_0(t)\rangle \tag{46}$$

with the initial condition

$$|\Psi_0(-\infty)\rangle = |n_0(-\infty)\rangle \equiv |N\rangle$$
 (47)

After the cycle, i.e., at $t = +\infty$, $|\Psi_0\rangle$ will have returned only approximately to $|N\rangle$, so a phase can be defined precisely by

$$\gamma \equiv \operatorname{Im} \log \langle N | \Psi_0(+\infty) \rangle - \gamma_d \tag{48}$$

The geometric phase $\gamma(C)$ (Eq. 13) is $\lim_{\epsilon \to 0} \gamma$. The aim is to obtain increasingly accurate approximations to $\gamma - \gamma(C)$. It is worth emphasizing that the non-aim is the determination of the nonadiabatic transition probability $1 - |\langle N|\Psi_0(+\infty)\rangle|^2$, because this is the usual objective of adiabatic theory, and that the non-method is perturbation theory, because this is the usual technique [30][49].

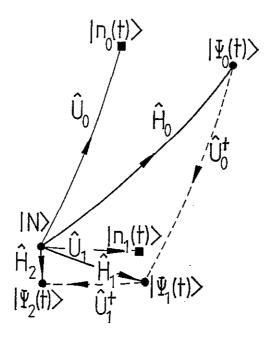


Figure 2. Renormalization in Hilbert space.

To explain the method used instead, we refer to Fig. 2. When ϵ is small we expect $|\Psi_0(t)\rangle$ to be close to $|n_0(t)\rangle$. This suggests that defining a unitary transformation $\hat{U}_0(t)$ by

$$|n_0(t)\rangle = \hat{U}_0(t)|N\rangle \tag{49}$$

will be useful. The inverse operator U_0^{\dagger} sends $|n_0(t)\rangle$ back to $|N\rangle$, that is, it freezes the moving eigenstate. Therefore \hat{U}_0^{\dagger} should almost freeze the evolving state $|\Psi_0(t)\rangle$, and so we define

$$|\Psi_1(t)\rangle \equiv \hat{U}_0^{\dagger} |\Psi_0(t)\rangle. \tag{50}$$

We are attempting to follow $|\Psi_0(t)\rangle$ by transforming to a moving frame. The Hamiltonian governing $|\Psi_1\rangle$ is

$$\hat{H}_1 = \hat{U}_0^{\dagger} \hat{H}_0 \hat{U}_0 - i \hat{U}_0^{\dagger} \dot{U}_0, \tag{51}$$

in which the second term is the quantum analogue of the inertial forces generated classically by transforming to a moving frame.

Now that the original problem has been reduced to one of the same form but involving $|\Psi_1\rangle$ and \hat{H}_1 instead of $|\Psi_0\rangle$ and \hat{H}_0 , it is natural to iterate the process by defining $|\Psi_2\rangle \equiv \hat{U}_1^{\dagger} |\Psi_1\rangle$, where \hat{U}_1^{\star} freezes the eigenstates $|n_1\rangle$ of \hat{H}_1 . This defines a renormalization map $\hat{H}_k \to \hat{H}_{k+1}$ in Hamiltonian space. The form of the map is simple when when written in a basis of initial states (which are unaffected by renormalization) and with the phases of the eigenstates chosen so that they are parallel-transported, i.e., $\langle n_k | \hat{n}_k \rangle = 0$:

$$\langle M|\hat{H}_{k-1}|N\rangle = E_k(n,t)\delta_{MN} - i\frac{\langle m_k(t)|\hat{H}_k(t)|n_k(t)\rangle}{E_k(m,t) - E_k(n,t)}(1 - \delta_{MN})$$
 (52)

The kth approximant $\gamma^{(k)}$ to the phase is obtained by neglecting the off-diagonal terms in \hat{H}_{k+1} . $\gamma^{(k)}$ is the sum of the phase anholonomies of the Hamiltonians \hat{H}_0 ... \hat{H}_k (arising from the continuation of $|n_k(t)\rangle$ from $t=-\infty$ to $t=+\infty$ and reflected as phase factors $\langle N|U_k(-\infty),N\rangle$), together with an additional term involving E_k [29]. (A contrary choice of phases, i.e., $|n_k(+\infty)\rangle = |n_k(-\infty)\rangle$, gives $\langle N|U_k(+\infty)|N\rangle = 1$, but now the diagonal terms in Eq. (52) contain extra terms $-i\langle n_k|\hat{n}_k\rangle$ and all corrections — including $\gamma^{(0)} = \gamma(C)$ as mentioned previously — appear dynamical.)

Each renormalization produces a new Hamiltonian which over $-\infty < t < +\infty$ traverses a loop in Hamiltonian space. If the renormalizations converged, successive loops would get smaller (by a factor ϵ each time). But this does not, and indeed cannot, happen. If it did, $\langle \Psi(-\infty)|\Psi(+\infty)\rangle$ would have modulus unity, contradicting the existence of transitions to other states. The accumulation of inertial forces in successive renormalizations defeats our attempts to follow the motion, which slips out of control, causing the scheme to diverge.

Nevertheless, the corrections generated by renormalization do get smaller at first, and enable γ to be determined with an error of order $\exp(-1/\epsilon)$, which occurs after $k \sim 1/\epsilon$ renormalizations. A detailed exploration [29] of 2-state systems (the simplest nontrivial case, for which the geometry of the loop map can be made explicit) reveals that the Hamiltonian loops (which lie on a 2-sphere) get smaller and then larger in a universal way (that is, almost always independent of the form of the initial loop).

This procedure is typical of asymptotic procedures and occurs also in the more usual adiabatic perturbation theory. It prompts interesting questions. What is the dynamical significance of the moving frame that produces the best approximant to γ , generated by $\hat{U}_{k-1/\epsilon}\hat{U}_{k-1}\cdots\hat{U}_0$? Can the exponential

residue $\gamma - \gamma^{(k)}$ be more closely approximated by generalizing the Borel (or some other) resummation method [47]?

It is instructive to illustrate adiabatic renormalization with the *classi-cal* problem which gave birth to the entire subject, namely the Ehrenfest-Einstein pendulum [31] whose frequency is slowly changed. Newton's equation is

$$\partial_t^2 x(t) + \omega^2(t) x(t) = 0 \tag{53}$$

in which the frequency $\omega(t)$ is a smooth nonzero function with $\omega(+\infty) = \omega(-\infty) \equiv \omega_{\infty}$. The same equation describ es the (time-independent) quantum mechanics of a beam of particles with energy E encountering a potential well or hill V(x) such that E > V(x) for all x.

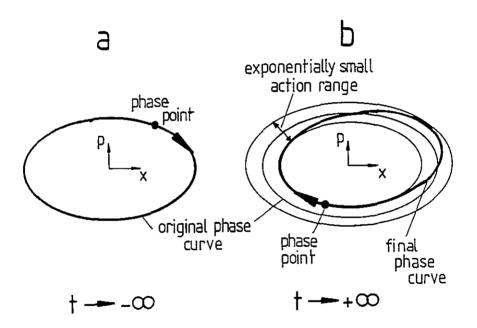


Figure 3. (a) Initial and (b) final phase portraits for slowly-altered pendulum.

Consider motion in the phase plane with variables x and $p = \dot{x}$. Initially, i.e., as $t \to -\infty$, each phase point moves round an ellipse with frequency ω_{∞} (Fig. 3a). The subsequent motion lies on a curve that at each instant approximates one of the elliptical contours of the Hamiltonian

$$H(x, p, t) = \frac{1}{2} \left[p^2 + \omega^2(t) x^2 \right]$$
 (54)

at that time. These subsequent ellipses have approximately the same area as the original one, because the adiabatically-conserved action is $area/2\pi$.

As $t \to +\infty$, then, the phase point is close to its original ellipse and we can ask: where is it on the ellipse, *i.e.*, what is its phase?

This would be a question about Hannay's angle were it not for the fact that this is a classical problem without anholonomy, so that the angle we seek consists entirely of nonadiabatic corrections. By identifying the solution of (53) with quantum transmitted and reflected waves, it can be shown that the oscillation which begins as

$$x + ip/\omega_{\infty} = A \exp\left\{-i\left(\int_{0}^{t} dt'\omega(t') + \sigma\right)\right\} \qquad (t \to -\infty) \qquad (55)$$

ends as

$$x + ip/\omega_{\infty} = A \exp\left\{-i\left(\int_{0}^{t} dt'\omega(t') + \sigma\right)\right\} \left[T^{-1} + RT^{-1}\exp(2i\sigma)\right]$$

$$(t \to +\infty) \qquad (56)$$

where A is a real constant and R and T are the complex quantal reflection and transmission coefficients.

Therefore the phase shift depends on the initial phase σ , but this dependence is slight because R is exponentially small in the slowness parameter ϵ (if ω depends on ϵt). In any case, we can define a phase by averaging over σ , with the exact result

$$\gamma \equiv -\frac{1}{2\pi} \int_{-\pi}^{\pi} d\sigma \lim_{t \to \infty} \left[\operatorname{Im} \log \left(x + i p / \omega_{\infty} \right) + \int_{0}^{t} dt' \, \omega(t') \right] = \operatorname{Im} \log T. \quad (57)$$

Thus 'Hannay's angle' is here the phase of the transmission coefficient. The final action I also depends on σ , but the range is $(I_{\text{max}} - I_{\text{min}})/I_{\text{initial}} = 4|R|/|T|^2$ which again is of order $\exp(-1/\epsilon)$; the whole initial ellipse of phase points evolves ultimately into one exponentially close to it and deforming periodically with frequency ω_{∞} (Fig. 3b). Newtonian renormalization of (53) is based on the transformation

$$x(t) \equiv \frac{x_1(t_1)}{\omega^{1/2}(t)}; \qquad t_1 \equiv \int_0^t dt' \, \omega(t')$$
 (58)

whose new coordinate satisfies

$$\partial_{t_1}^2 x_1(t_1) + \omega_1^2(t_1) x_1(t_1) = 0 (59)$$

where

$$\omega_1^2(t_1(t)) = 1 + \omega^{-3/2} \partial_t^2 \omega^{-1/2}. \tag{60}$$

Clearly $\omega_1 \approx 1$ if ω varies slowly.

Renormalization consists of iterating this transformation, the aim being to freeze the frequency. The kth approximant for γ is obtained by approximating $\omega_{k+1} \approx 1$, so

$$\gamma^{(k)} = \int_{-\infty}^{\infty} (dt_{k+1} - \omega(t) dt) = \int_{-\infty}^{\infty} dt \, \omega \left(\prod_{j=1}^{k} \omega_j - 1 \right)$$
 (61)

Thus

$$\gamma^{(0)} = 0 \qquad \text{(no anholonomy in this problem)}$$

$$\gamma^{(1)} = \int_{-\infty}^{\infty} dt \, \omega(t) \Big(\omega_1(t_1(t)) - 1 \Big)$$
(62)

etc. $\gamma^{(1)}$ is of order ϵ .

An equivalent *Hamiltonian* renormalization is produced by iteration of the canonical transformation generated by

$$S(x, p_1, t) = x p_1 \omega^{1/2} - x^2 \partial_t \omega / 4\omega. \tag{63}$$

This gives

$$x_1 = x \omega^{1/2}; \qquad p_1 = p \omega^{-1/2} + x \partial_t \omega / 2\omega^{3/2}$$
 (64)

and hence the transformed Hamiltonian

$$\overline{H}(x_1, p_1, t) = H + \partial_t S = \frac{1}{2}\omega(t) \left(p_1^2 + \omega_1^2 x_1^2 \right)$$
 (65)

where ω_1 is given by (60). Rescaling time to t_1 as defined in (58) now gives

$$H_1(x_1, p_1, t_1) = \frac{1}{2} \left(p_1^2 + \omega_1^2(t_1) x_1^2(t_1) \right)$$
 (66)

which is the first renormalization of the original Hamiltonian (54). The aim of subsequent renormalizations is to freeze the Hamiltonian into one whose contours are circles.

I have expressed these classical iteration schemes in terms of the renormalization of Newton's or Hamilton's equations in order to illustrate the idea behind the quantum renormalization described earlier. But they can be shown to be equivalent to the following fairly conventional WKB-like [32] procedure (to be contrasted with an unconventional WKB analysis by Wilkinson [45] which, unlike this one, does involve anholonomy). Write the exact solution of Eq. (53) as

$$x(t) = \Omega^{-1/2}(t) \cdot \exp\left\{i \int_0^t dt' \, \Omega(t')\right\}. \tag{67}$$

Then the 'frequency' $\Omega(t)$ satisfies

$$\Omega^{2}(t) = \omega^{2}(t) + \Omega^{1/2}(t) \,\partial_{t}^{2} \Omega^{-1/2}(t). \tag{68}$$

In terms of Ω , the phase shift is, exactly,

$$\gamma = \int_{-\infty}^{\infty} dt \left[\Omega(t) - \omega(t) \right]. \tag{69}$$

Successive approximants are obtained by the iteration

$$\Omega^{(0)} = \omega \; ; \qquad \Omega^{(k-1)} = \left[\omega^2 + (\Omega^{(k)})^{1/2} \, \partial_t^2 (\Omega^{(k)})^{-1/2} \right]^{1/2} . \tag{70}$$

The inevitability and universality of the divergence of these schemes can be demonstrated by considering high-order iterations of Eq. (60), for which

$$\omega_k(t) \equiv 1 + \delta_k(t) \tag{71}$$

and $\delta_k \ll 1$. Then $t_{k+1} \approx t_k$ (cf.Eq. (58)), and Eq. (60) can be written approximately as

$$\delta_{k+1}(t) \approx -\frac{1}{4}\partial_t^2 \delta_k(t). \tag{72}$$

The asymptotics of this recursion as $k \to \infty$ can be estimated by Fourier analysis, on the assumption that $\delta_0(t)$ is a real function of $\tau \equiv \epsilon t$, analytic in a strip about the real τ axis with its nearest singularities at $\tau_1 \pm i\tau_2$. Then with $\xi \equiv (\epsilon t - \tau_1)/\tau_2$ it is possible to show that

$$\delta_k(t) \xrightarrow[k \to \infty]{} \left[\frac{A\epsilon^{2k}(2k)!}{4^k \tau_2^{2k+1}} \right] \left[\frac{\cos\left\{ (2k+1)\cos^{-1}(1+\xi^2)^{-1/2} \right\}}{(1+\xi^2)^{k+1/2}} \right]$$
(73)

where A is a constant.

The first factor in (73) shows the divergence: $\epsilon^{2k}(2k)$! decreases until $k \sim \tau_2/\epsilon$, when $\delta_k \sim \exp(-2\tau_2/\epsilon)$, and then increases until $\delta_k \sim 1$, when the scheme breaks down. The second factor is the universal function describing the asymptotic 'frequency.'

7. Historical Remarks

First I consider the important special case where the transported states $|\psi\rangle$ can be represented by wavefunctions that are real. Then the only possible phase factors associated with a circuit C are ± 1 . It follows [7] from the result (22) for spins that the factor is -1 when C encloses a degeneracy X^* of the spectrum to which $|\psi\rangle$ belongs; otherwise, it is +1. The peculiarity of this case is that parallel transport (10) is the only possible smooth continuation law, rather than a mathematically natural choice, concordant with quantum dynamics, from a infinity of possibilities.

Eigenfunctions can always be made real if their Hamiltonian matrix is real symmetric rather than complex Hermitian (this is the case when there is (bosonic) time-reversal symmetry [34]). Thus the phase law states

that an eigenfunction of a real symmetric matrix depending on parameters changes sign under smooth continuation round a degeneracy. This result is so simple – it holds even for 2×2 matrices – as to deserve mention in elementary expositions of matrix theory, but I have not found it in any such text. Arnold [14] is aware of the sign change, and attributes it to Uhlenbeck [35] in 1976. It was already known to theoretical chemists: Herzberg and Longuet-Higgins [36] gave an explicit statement in 1963. But the sign change (for 2×2 matrices) was implicit in work of Darboux [37] as long ago as 1896. This concerns the differential geometry of surfaces, and is worth describing.

Darboux considered a curved surface described locally by its deviation $z(X_1, X_2)$ from the plane $X = (X_1, X_2)$. Then the 2×2 real symmetric curvature matrix at X is

$$H_{ij}(X) = \partial_i \partial_j z(X). \tag{74}$$

The two eigenvalues are the principal curvatures at X, and the corresponding eigenvectors give the (orthogonal) directions of the lines of curvature at X. Degeneracies are *umbilic points*, where the surface is locally spherical (two curvatures equal). Umbilics are singularities of the net of curvature lines. The sign-change rule states that a line of curvature turns by π in a circuit of an umbilic: the Poincaré index of the tensor field (74) is $\pm \frac{1}{2}$. Fig. 4 shows how this happens for the three generic patterns [38][39] of curvature lines near an umbilic; the star has index $-\frac{1}{2}$, and the lemon and monstar have index $+\frac{1}{2}$. Star and lemon singularities occur as disclinations in liquid crystals [48].

The full phase — rather than the impoverished special case of the sign change for real matrices — was anticipated at least twice. First, in the mid-1950's, Pancharatnam [20][21][40] studied the 2-state Hermitian case in the context of the polarization states of light travelling in a fixed direction. The parameter space is the surface of the Poincaré sphere. Pancharatnam introduced the useful idea of defining two different states $|1\rangle$ and $|2\rangle$ as 'in phase' if the intensity of their superposition is maximal, a condition equivalent to their overlap $\langle 1|2\rangle$ being real and positive. This defines a connection between the corresponding parameters X_1 and X_2 as the state $|2\rangle$ obtained from $|1\rangle$ by phase-preserving transport along the shorter geodesic arc between X_1 and X_2 . He discovered that the connection is nontransitive: a circuit $X_1X_2X_3X_1$ produces a state differing from $|1\rangle$ by precisely the same phase anholonomy [21] (minus half the solid angle of the circuit) as that given by parallel transport.

Second Mead [24] and Mead and Truhlar [42], studying adiabatic theory for molecules, made two important advances. They showed how the sign-change rule for degeneracies would induce modifications in the nuclear dynamics and hence change the vibration-rotation spectrum. And they realized that in the absence of time-reversal symmetry the nuclear dynamics would be influenced by the vector potential (39) and the corresponding 'magnetic' field (41), for which they gave a general formula.

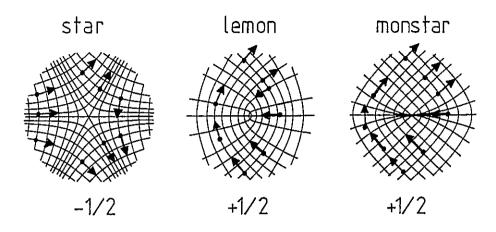


Figure 4. The generic patterns of lines of curvature near an umbilic point on a surface, illustrating the reversal $(\pm 1/2 \text{ index})$ round the singularity.

My involvement with this subject began in 1979 with the appreciation [43] that degeneracies play a part in determining the fine-scale statistics of energy levels of quantum systems whose classical counterparts are nonintegrable. The systems under study possessed time-reversal symmetry and so their states should change sign round degeneracies. Seeking to display some degeneracies and their sign changes, M. Wilkinson and I [44] made a detailed investigation of the spectra of vibrating triangles as a function of angles (two parameters).

After a seminar reporting this work in the spring of 1983 at the Georgia Institute of Technology, R. Fox asked me, "what happens to the sign change if a magnetic field is switched on?", and this question led directly to the discovery of the phase and its 2-form several weeks later. Only when the work was written in first draft was I made aware (by E.Heller) of the papers by Mead and Truhlar. In August 1983, after my paper [7] had been submitted for publication, I described the phase to B.Simon, who instantly saw its relationship to Hermitian line bundles and Chern classes. His paper [10] directed many people towards this subject, thereby provoking the considerable activity of which this book is a partial record. But thanks to a referee's delay and an accident of astronomy, his paper appeared in 1983, mine in 1984.

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