ANTICIPATIONS OF THE GEOMETRIC PHASE

The notion that a quantum system's wavefunction may not return to its original phase after its parameters cycle slowly around a circuit had many precursors—in polarized light, radio waves, molecules, matrices and curved surfaces.

Michael Berry

In science we like to emphasize the novelty and originality of our ideas. This is harmless enough, provided it does not blind us to the fact that concepts rarely arise out of nowhere. There is always a historical context, in which isolated precursors of the idea have already appeared. What we call "discovery" sometimes looks, in retrospect, more like emergence into the air from subterranean intellectual currents.

The geometric phase, whose discovery I reported early in 1983, is no exception to this rule.[1] The paper was about quantum systems forced round a cycle by a slow circuit of parameters that govern them; it gave rise to a number of applications and several generalizations, documented in a series of reviews and books.[2–5] My purpose here is to look back at some early studies that with hindsight we see as particular examples of the geometric phase or the central idea underlying it.

Parallel transport

First I need to explain this central idea. It is the geometric phenomenon of anholonomy resulting from parallel transport. This is a type of nonintegrability, arising when a quantity is slaved to parameters so as to have no local rate of change when those parameters are altered, but nevertheless fails to come back to its original value when the parameters return to their original values after being taken round a circuit.

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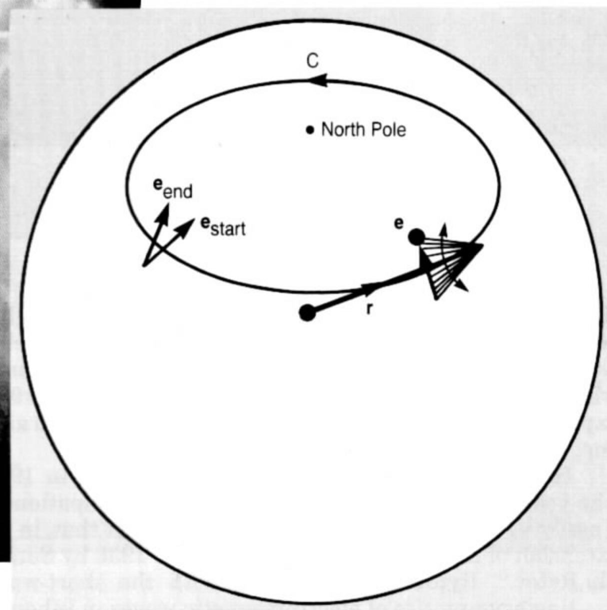
A physical example of this "global change without local change" is the Foucault pendulum (figure 1), whose direction of swing, described by a unit vector **e**, is slaved to the local vertical, described by the radial unit vector **r**. The slaving law is parallel transport, which means that the direction of swing does not rotate about the vertical—that is, **e** has no component of angular velocity along **r**. However, in spite of never being rotated, **e** does not return to its original value when, after a day, **r** has completed a circuit C (here a circle of latitude). The anholonomy is the angle between the initial and final swing directions **e**, and is equal to the solid angle subtended at the Earth's center by C.

A note about terminology: Although the anholonomy of parallel transport of a vector on a curved surface was known to Gauss nearly two centuries ago, the word seems to have entered the literature through the study of mechanics in the presence of constraints. A constraint is holonomic if it can be integrated and thereby can reduce the number of degrees of freedom, as with a rolling cylinder. Otherwise, it is nonholonomic (or nonholonomous, or anholonomic), as with a rolling disk, which can sway from side to side. According to the *Oxford English Dictionary* the word was first used by Hertz in 1894. Nowadays the concept of anholonomy is familiar to geometers, but they often call it "holonomy," a reversal of usage I consider a barbarism.

The geometric phase can be regarded as anholonomic for the parallel transport of quantum states. Mathematically, quantum states are represented by unit vectors in Hilbert space. Although these unit vectors are complex,



Foucault pendulum at Griffith Observatory in Los Angeles, and diagram showing its anholonomy. The direction of swing does not return to its initial value when the pendulum completes its one-day trip around a circle of latitude. (In the diagram, the direction of swing **e** is parallel-transported around the diurnal circuit *C* by the local vertical **r**.) At the latitude of Los Angeles, the direction of swing comes back to its original value after 42 hours, and so the pit is marked off in 42 segments. (Courtesy of Edwin Krupp, Griffith Observatory.) **Figure 1**

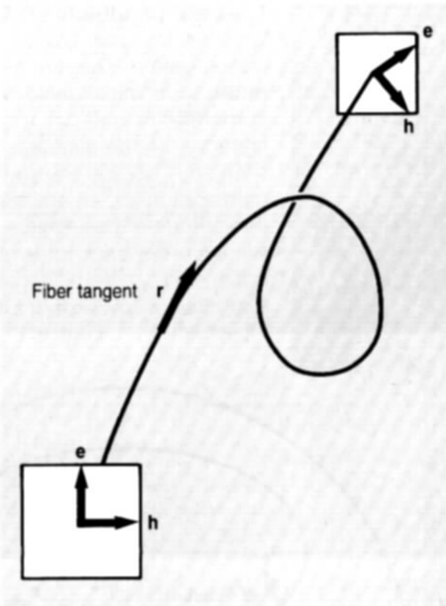
parallel transport can still be defined. A natural way to implement it is by a slow cycle C of parameters in the Hamiltonian governing the evolution of the system according to Schrödinger's equation. The quantum adiabatic theorem guarantees that if the system starts in the instantaneous eigenstate labeled n, it will still be in the state n at the end of the cycle C. However, the *phase* of the state vector need not, and usually does not, return. Part of this change—the geometric phase—is the manifestation of anholonomy.

To give an account of the earlier work, I have first to describe the geometric phase for spinning particles. This concerns a spinor state corresponding to a definite value s (integer or half-integer) for the component of spin along some direction **r**. An example is a spin eigenstate ($s = \pm \frac{1}{2}$) of a neutron in a magnetic field with direction **r**. If the direction is cycled, that is, taken round a closed curve C on the unit **r** sphere, the state acquires a geometric phase equal to $-s$ times the solid angle subtended by C at the center of the sphere. As is well known, the spin-$\frac{1}{2}$ case is isomorphic to the general quantum two-state system, where the Hamiltonian is a 2×2 complex Hermitian matrix.

Coiled light

Raymond Y. Chiao, Akira Tomita and Yong-Shi Wu were quick to apply the spin phase to optics, by regarding a light beam as a stream of photons with quantization direction **r** along the direction of propagation.[2] The two states, $s = \pm 1$, correspond to left- and right-handed circularly polarized light. To cycle **r** they therefore had to cycle the direction of propagation, which they accomplished by sending the light along optical fibers that were coiled into paths such as helices, and for which the initial and final tangent directions **r** were parallel. An obvious way to observe the geometric phase would be to split a beam of (say) left circularly polarized light into two coherent beams, send them along two oppositely coiled fibers, recombine them and detect the resulting opposite geometric phases by interference. Instead, Chiao, Tomita and Wu performed the simpler experiment of sending a single beam of *linearly* polarized light along a single fiber. The initial linear polarization is a particular superposition of the $s = +1$ and $s = -1$ states, which acquire opposite phases after passage through the fiber and so emerge in a different superposition, corresponding again to linear polarization, but now in a different direction. (The "interference" and "superposition" techniques correspond to two different general methods for detecting the phase, employing, respectively, one state and two different Hamiltonians or two states and one Hamiltonian.)

One manifestation of the geometric phase for light is therefore a rotation of the direction of polarized light (figure 2) after it has traveled along a coiled optical fiber. The angle of rotation is equal to the solid angle through which the fiber tangent **r** has turned, implying that the polarization has been parallel-transported. Chiao and his coworkers themselves pointed out that this appears to be a phenomenon of classical optics, which although originating in the quantum mechanics of spinning photons survives the classical limit $\hbar \to 0$ up to the level described by Maxwell's equations. They did not, however, show how



Rotation of linear polarization by parallel transport along a coiled optical fiber. The vectors **e** and **h** represent the electric and magnetic fields, respectively. **Figure 2**

the rotation of polarization is contained in Maxwell's equations; nor had J. Neil Ross of the Central Electricity Generating Board Laboratories, in Leatherhead, England, who had demonstrated the rotation earlier, in a 1984 experiment. (Ross implicitly assumed the parallel transport law.)

However, in a remarkable paper, published in 1941 (the year I was born) and the first of our "anticipations," Vassily V. Vladimirskii had, in effect, done just that, in an extension of an earlier paper published in 1938 by Sergei M. Rytov.[6] Rytov was concerned with the short-wave limiting asymptotics of electromagnetic waves in inhomogeneous media. He was dissatisfied with the conventional derivations of the generalized Snell refraction law of geometrical optics (ray curvature is equal to the component of grad[log(refractive index)] perpendicular to the ray), because this ignores the vector nature of light waves: There had to be a transport law for the directions **e** and **h** of the electric and magnetic fields. He showed that the law is parallel transport—of the orthogonal triad consisting of **e**, **h** and the ray direction **r**.

Vladimirskii's contribution—surprisingly modern in tone—was to show that Rytov's law is nonintegrable and implies the solid-angle law for the rotation of polarization. Vladimirskii pointed out one consequence of his analysis: Observation of polarization rotation of an outgoing ray relative to a parallel incident ray does not imply anisotropy (or chirality) of the intervening medium, because it could result from ray curvature induced by inhomogeneity of the medium. He did not state that parallel transport of the fields implies phase anholonomy for circularly polarized rays, but Rytov came close, remarking that it implies different phase velocities for the two circular polarizations.

In essence, the theory that Vladimirskii and Rytov developed contains the explanation of the experiments of Chiao's group. Strictly speaking, however, Vladimirskii and Rytov's analysis cannot be invoked, because those experiments employed monomode fibers, which are too thin for geometrical optics to be validly applied. It is necessary to use the full Maxwell equations, either in a modal analysis[7] or, when recast as a Schrödinger-type spinor equation, to enable immediate application of the spin-1 geometric phase formula.[5]

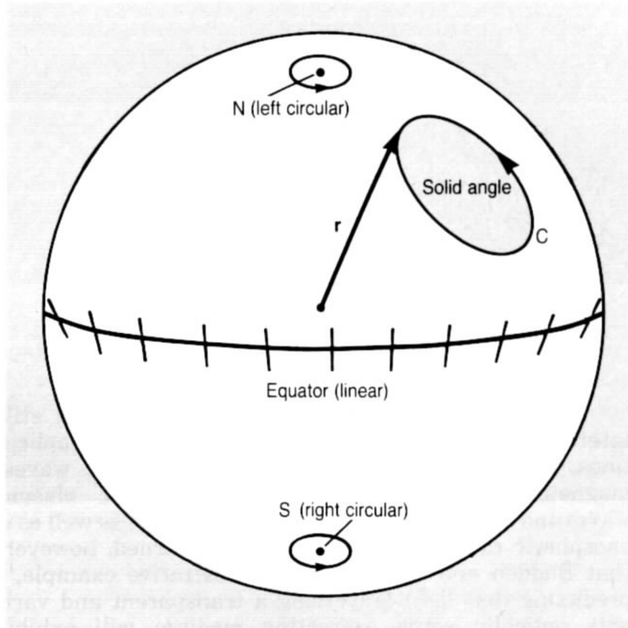
It is worth pausing to note the political circumstances in which Vladimirskii worked. In 1941, a few months after he submitted his paper, the Soviet Union was plunged into the turmoil of World War II by Hitler's sudden invasion.

Polarization cycles

In a different application to optics, I considered not light with a fixed state of polarization (circular, for example) and changing direction, but the opposite, namely light traveling in a fixed direction with a slowly changing state of polarization.[8] A way to accomplish this, and thereby generate a geometric phase, would be through a transparent medium that was both anisotropic and chiral (such as a liquid in strong electric and magnetic fields) and so possessed both birefringence and gyrotropy. These properties would be reflected in the complex Hermitian dielectric tensor of the medium, which could be varied along the beam and then brought back to its original form. (Actually what is relevant is only the 2×2 matrix representing the components of the inverse of this tensor perpendicular to the beam.)

This too had been anticipated, in a strikingly original paper published 30 years before by S. Pancharatnam of Bangalore.[9] He was investigating the interference patterns produced by plates of anisotropic crystal, and found existing theory inadequate to explain what he saw. In particular, he needed to define how two beams in different polarization states (linear and elliptic, for example) could have the same phase. He did this by considering the intensity of the wave obtained by coherent linear superposition of the two beams. As the phases of the individual beams are varied, this intensity waxes and wanes. When it is maximum, the two beams are defined as being "in phase." The two beams could represent successive states in the polarization history of a single beam, so this procedure also enabled him to define how a beam can preserve its phase while its polarization state is altered (not necessarily slowly).

Pancharatnam then made the important observation that this law of phase preservation is *nontransitive*. Thus a beam may start out with a polarization 1, which is altered first to polarization 2, in phase with 1, then to 3, in phase with 2, and then back to 1, in phase with 3; and yet the final polarization-1 beam need not have the same phase as the initial polarization-1 beam, in spite of the fact that all three local phase changes were zero. To calculate the phase change, he represented states of polarization as points on the "Poincaré sphere" (see figure 3). In this picture, the poles represent left- and right-handed circular polarization; points on the equator represent linear polarizations (with the direction rotating by 180° in a 360°



Poincaré sphere of polarization states **r**. The phase change associated with a circuit C of polarization states is half the solid angle subtended by C at the center of the sphere. **Figure 3**

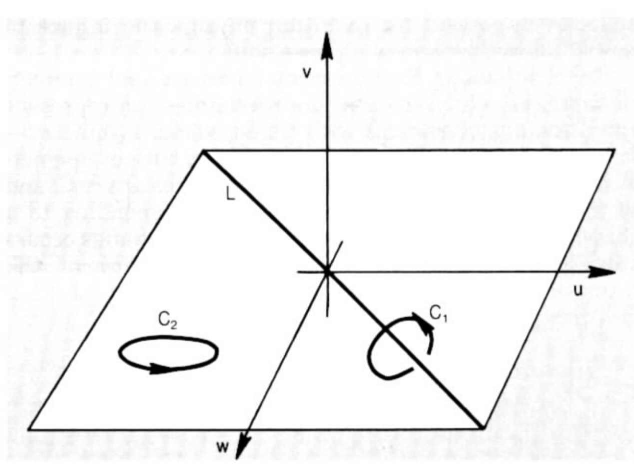
circuit, because two polarization orientations differing by 180° are the same); and all other points represent elliptic polarizations. The path 1231 is a circuit C on the sphere, and Pancharatnam discovered that the associated phase change is half the solid angle subtended by C at the center of the sphere.

Clearly, Pancharatnam discovered what we would now call the geometric phase for polarization circuits of light. To make the connection with the way we see things nowadays, it is first necessary to know that the polarization associated with the point on the Poincaré sphere indicated by the unit vector **r** (that is, the corresponding transverse electric field represented by the complex unit vector **e**) is represented by the complex eigenvector of $\mathbf{S}\cdot\mathbf{r}$, where **S** is the vector of three 2×2 Pauli spin-½ matrices.[10] (The components of **r** are the Stokes parameters of the polarization.) This relation between polarizations and quantum states of spin-½ particles—that is, with two-state systems—is unsurprising, because any polarization of light traveling in a fixed direction is a superposition of two basis polarizations—for example, left and right circular, or horizontal and vertical linear. The crucial step is now to demonstrate that parallel transport of these eigenvectors is equivalent to Pancharatnam's phase preservation rule for the associated polarizations. The "half the solid angle" rule follows at once from the spin-½ analogy.

Pancharatnam was a nephew of C. V. Raman, and so belonged to the distinguished dynasty that includes the astrophysicist S. Chandrasekhar, the liquid crystal physicist S. Chandrasekhar, the crystallographer S. Ramaseshan and the radioastronomer V. Radhakrishnan. When Pancharatnam wrote about polarized light, he was only 22 years old. In spite of this brilliant beginning, his story ended sadly, with his untimely death at the age of 35.

While writing this article I discovered some remarkable papers written in 1975 by Martin S. Smith and Kenneth G. Budden,[11] who although unaware of the earlier works by Vladimirskii and Pancharatnam nevertheless provide a more general viewpoint into which these fit as special cases. Budden and Smith were studying the propagation of short radio waves in the ionosphere, where the "ray" or "WKB" approximation is appropriate. Such wave fields are dominated by a complex exponential factor whose phase is the familiar optical path length—the integral of the local wavenumber. They called this path integral "phase memory" because it depends on the properties of the medium—the atmosphere—along the entire propagation path. Thus it is nonintegrable, in contrast to the wave amplitude, which in the simplest theory is a "local" factor depending only on the properties (such as refractive index) at the ends of the ray.

Budden and Smith's contribution was to show that in all but a few cases the simplest theory is wrong, because there is an additional factor, which they called "additional memory," whose exponent also depends nonintegrably on the propagation path. The additional memory may be real or complex and so can contribute nonlocally to the phase or the amplitude. They gave a theory covering a very general class of waves, described by vectors whose evolution along the ray is driven by a matrix embodying the properties of the medium. Although they did not consider cycles of the medium parameters, their general formula expressing the additional memory as an integral along the ray can be shown to be exactly the one we are now familiar with in quantum mechanics, which can be viewed as a special case where the driving matrix is Hermitian and the ray parameter is time.[12]



Line of degeneracies of elements of a real symmetric 2×2 matrix. The circuit C_1 encloses the line L of degeneracies and so generates a geometric sign change; C_2 does not enclose L, and so does not generate such a change. **Figure 4**

As well as including technicalities that are still interesting today,[12] Budden and Smith gave many applications, demonstrating phase memory in seismic waves, magnetohydrodynamic waves, electroacoustic plasma waves and atmospheric acoustic gravity waves as well as ionospheric radio waves. (Readers are warned, however, that Budden and Smith's initial illustrative example,[11] predicting that light traversing a transparent and variably optically active refracting medium will exhibit additional memory, is wrong because they employ an unphysical constitutive relation. When this is corrected, the additional memory is canceled by a part of the ordinary memory.[12])

Degeneracy

The existence of geometric phases implies that quantum eigenstates are not single-valued under continuation of parameters in the Hamiltonian. Thus expressed, phase anholonomy appears to be a rather subtle property, especially when contrasted with the more familiar single-valued-ness demanded of wavefunctions under continuation of position coordinates, which is necessary to get quantized energy levels (in the harmonic oscillator, for example). However, when detached from its original quantum mechanical context, the geometric phase can be regarded as an expression of a simple property of matrices that depend on parameters—that is, of families of matrices: Their eigenvectors are not single-valued when parallel-transported via changes of the parameters. After a parameter circuit C, the eigenvectors do not return to their original values. In the class of complex Hermitian matrices important for quantum physics, the failure to return takes the form of a phase shift.

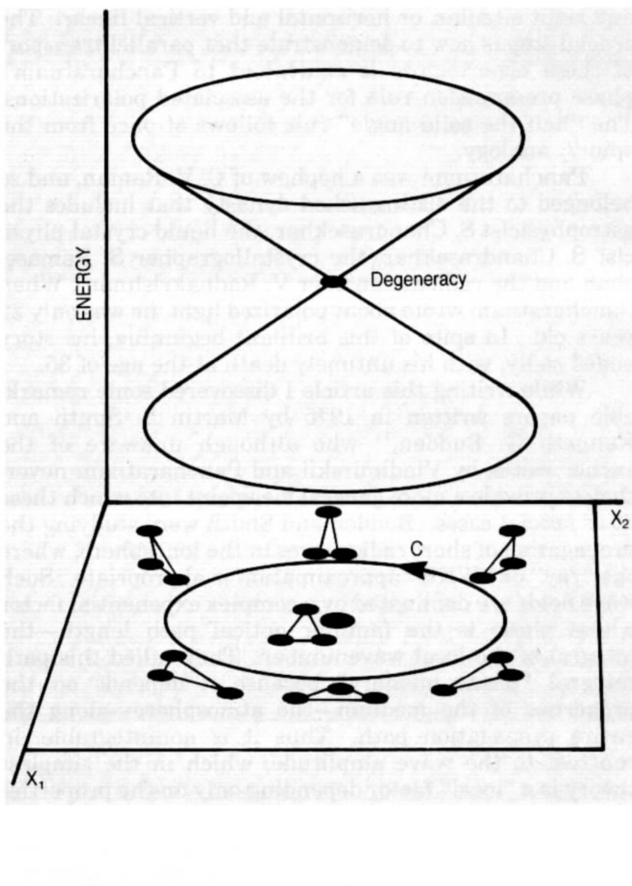
Special among Hermitian matrices are real symmetric matrices, which in quantum mechanics can represent Hamiltonians of systems with time-reversal symmetry—for example, charged particles in electric, but not magnetic, fields. The eigenvectors of these matrices are real, and so the only phase anholonomy is π, corresponding to a change of sign of the eigenvectors. The sign change occurs only if the circuit C encloses a degeneracy of the transported state. The simplest case is that of 2×2 matrices

$$\mathbf{M} = \begin{pmatrix} u & v \\ v & w \end{pmatrix}$$

Here degeneracies in the u,v,w parameter space correspond to the line $v = 0$, $u = w$, and so there is a sign change in the eigenvectors only if C encloses this line (see figure 4).

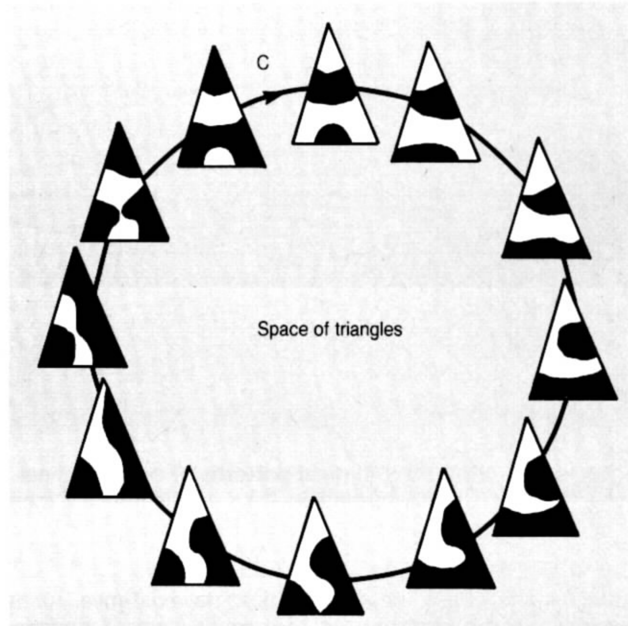
Such a simple property—even of 2×2 matrices—was not well known in 1983. I could find no reference to it in textbooks of matrix theory (and would welcome information about any). Nevertheless, it was known, in particular to quantum chemists studying the vibrations and rotations of molecules. In the Born–Oppenheimer (adiabatic) approximation, the coordinates of the nuclei are regarded as parameters, to which quantum states of the electrons are slaved. Nuclear configurations with symmetry can give rise to degeneracy of the electronic energies. In 1958, H. Christopher Longuet-Higgins, Uno Öpik, Maurice H. L. Pryce and Robert A. Sack noticed that in the solution of a particular model the electronic wavefunctions changed sign when the nuclear coordinates made a circuit of the symmetric (degenerate) configuration (see figure 5).[13] This is the π anholonomy of real symmetric matrices, recognized as a general phenomenon by Gerhard Herzberg and Longuet-Higgins[14] in 1963.

Longuet-Higgins and his coworkers realized that the



Nuclear coordinate circuit. The circuit C is in the space of nuclear coordinates X of triatomic molecules. The circuit surrounds the equilateral molecule, for which there is an energy level degeneracy (at the conical intersection). **Figure 5**

Drumhead-shape circuit. The circuit C is in the space of boundary shapes of triangular drums, and surrounds a shape for which the vibration mode is degenerate. (The shapes look the same because the circuit is small.) The dark and light areas of the vibrating drums correspond to the conventional labels + and −. Note that the vibrations in the triangles at the beginning and end of the circuit (the triangles on either side of the arrow) differ only in phase, by 180°. **Figure 6**



sign change has physical consequences when the nuclear coordinates are themselves quantized instead of being regarded as externally specified parameters: The vibration–rotation energies have half-odd-integer quantum numbers, rather than the usual integer ones. They remarked, "This half-oddness is at first sight strange, but may be understood by noting that [around a circuit] the electronic factor in the wavefunction will be multiplied by −1, so that the angular part of the nuclear factor must do likewise if the total wavefunction is to be single-valued." This is the phenomenon of pseudorotation, which has been of considerable interest recently.[15]

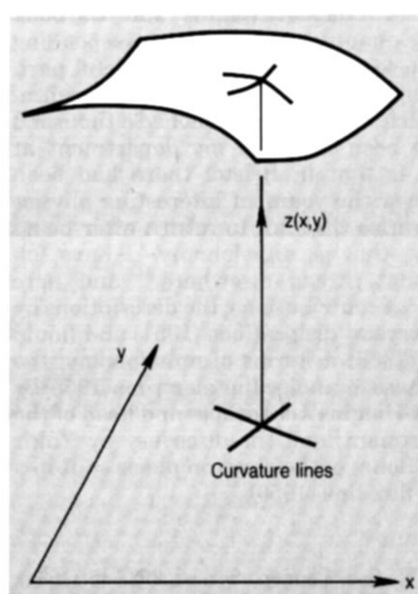
Among mathematicians, the sign change was also known. In his celebrated text on classical mechanics, Vladimir I. Arnold describes it for a modal eigenfunction of a vibrating membrane, or drum, whose boundary is varied round a circuit C in the space of boundary shapes surrounding a shape for which the mode is degenerate.[16] For any point on the circuit, the drum eigenfunction is divided by nodal lines into regions that may be conventionally labeled + and −. Around the circuit, the nodal lines move over the domain and collide, disconnect and reconnect so as to change the + regions into − regions continuously, and vice versa, as figure 6 illustrates for a set of triangular membranes. Arnold traces the sign change to a 1976 paper of Karen Uhlenbeck,[17] but, as we have seen, the chemists knew about it in 1958.

Curved surfaces

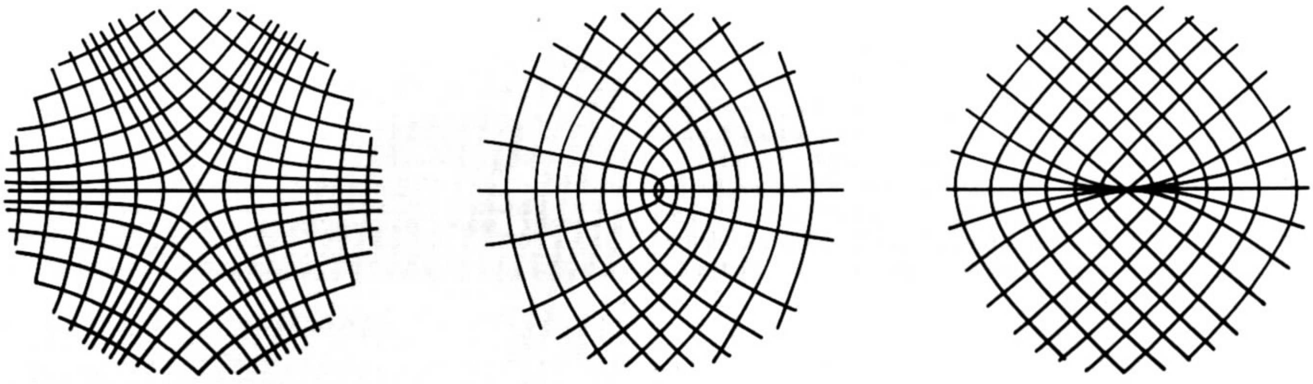
The 2×2 sign change is much older. I do not know when this was first recognized as a property of matrices, but it is implied by a result in Gaston Darboux's monumental 1896 treatise on the differential geometry of curved surfaces.[18] This might be the first example of phase anholonomy, albeit the rudimentary π case. Locally, a smooth surface can be specified by its deviation $z(x,y)$ from a plane, as figure 7 indicates. From this function one can form the 2×2 real symmetric Hessian (curvature) matrix $\mathbf{H}(x,y)$ of second derivatives, and x and y can be regarded as parameters. The eigenvalues of $\mathbf{H}$ are the principal curvatures of the surface at (x,y)—that is, the greatest and least curvatures of normal sections through the surface at (x,y). The corresponding eigenvectors are the directions of these special cuts, and are orthogonal. An unusual feature of this example is that the eigenvectors can be considered to lie in the parameter space, as well as being functions of the parameters. Degeneracies (x,y) correspond to equality of the two curvatures—that is, to "umbilic points," where the surface is locally spherical rather than ellipsoidal or saddle-shaped as it is at typical points. Umbilics are singularities of the orthogonal net of curvature lines. The sign change characterizes such a singularity by a reversal of the curvature directions in a circuit of it. Alternatively stated, the Poincaré index, or signed number of rotations associated with an oriented circuit, of the field of curvature lines near an umbilic is $+\frac{1}{2}$ or $-\frac{1}{2}$.

A complete characterization of the geometry of an umbilic is complicated.[19] Figure 8 shows the three typical patterns of curvature lines, one of which (the "star") has index $-\frac{1}{2}$ and the others of which (the "lemon" and the "monstar") have index $+\frac{1}{2}$. The half-integer index is typical of singularities of line fields (which do not have arrows), such as those associated with eigenvectors of families of matrices, in contrast to the integer indices of vector fields (which do have arrows). The star and lemon singularities are familiar, with one of the two orthogonal sets of lines deleted, as disclinations in the molecular line fields of liquid crystals,[20,21] and in fingerprints.

In 1976, Anthony J. Stone[22] generalized the connection between degeneracy and the sign change[13,14] by considering complex Hamiltonians. He realized that in this general case, where the wavefunctions are also complex, an arbitrary phase, not just π, could be generated by taking a system round a circuit C. Without giving a for-



Curvatures at a point on a surface. Locally, a smooth surface can be specified by its deviation $z(x,y)$ from a plane. **Figure 7**



The three typical patterns of curvature lines near an umbilic singularity, where the surface is locally spherical. The star has index $-\frac{1}{2}$. The lemon and monstar have index $+\frac{1}{2}$. **Figure 8**

mula for the phase, he showed how its existence, for a succession of circuits that together cover a closed surface, could provide a topological indicator of the presence of a degeneracy.

Another anticipation, of which I was regrettably unaware when writing my original paper,[1] was the important work by C. Alden Mead and Donald G. Truhlar in 1979, containing two developments in the theory of general complex Hamiltonians.[23] This theory would apply, for example, to systems with magnetic fields, which do not have time-reversal symmetry. Like Longuet-Higgins and his coworkers, Mead and Truhlar were studying molecules in the Born–Oppenheimer approximation. The first of the developments was that they not only realized that the electronic states must acquire a phase when the nuclear coordinates are cycled, but they also gave a general formula for the phase in the case of infinitesimal circuits. Second, they discovered another role for the expression whose line integral around the circuit generates the phase: It is the potential of an effective "gauge force" contributing to the dynamics of the nuclei. The effect of this force is to modify the nuclear vibration–rotation spectrum, as in the special case of pseudorotation mentioned earlier.

As elaborated elsewhere,[24] in 1983 I was familiar with the π phase shifts of Longuet-Higgins and Darboux through studies of the quantum mechanics corresponding to classical chaos, where degeneracies play a useful part. In retrospect it now appears natural that the generalization to the full geometric "phase that launched a thousand scripts" should have been made in my department at Bristol. The reason is that in Bristol there had been several discoveries, over the years, of interesting physics associated with quantities that fail to return after being taken round circuits—that is, anholonomy. I have followed that intellectual thread elsewhere,[21] and here simply list some of those contributions: the descriptions by F. Charles Frank of crystal dislocations (1951) and liquid crystal disclinations (1958) in terms of anholonomy; the description of the π phase for molecular electrons (1958) by Pryce, one of Longuet-Higgins's coauthors and head of the Bristol physics department; and the discovery by Yakir Aharonov and David Bohm of the electron phase shift in a circuit of a magnetic flux line (1959).

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