WAVE GEOMETRY: A PLURALITY OF SINGULARITIES

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ABSTRACT

Five interconnected wave singularities are discussed: *phase monopoles*, at eigenvalue degeneracies in parameter space, where the 2-form generating the geometric phase is singular; *phase dislocations*, at zeros of complex wavefunctions in position space, where different wavefronts (surfaces of constant phase) meet; *caustics*, that is envelopes (foci) of families of classical paths or geometrical rays, where real rays are born violently and which are complementary to dislocations; *Stokes sets*, at which a complex ray is born gently where it is maximally dominated by another ray; and *complex degeneracies*, which are the sources of adiabatic quantum transitions in analytic Hamiltonians.

1. Introduction

A rather old-fashioned view of quantum mechanics is that it is an application of the physics of waves. A not so old-fashioned way to get interesting physics out of mathematical objects is by studying their singularities. Here I will combine these two ideas and describe a variety of singularities (in several spaces) in waves, quantum and otherwise. This leads to an unorthodox way of thinking about waves, apparently very different from, but actually complementary to, the usual ones based on wave equations, Fourier analysis, etc. It is appropriate to be talking about it at a meeting celebrating the 30th birthday of the Aharonov-Bohm effect[1], for at least two reasons.First, their effect exemplifies several of the ideas I will describe. Second, it lies squarely in the geometrical tradition of the physics department at Bristol University where Aharonov and Bohm discovered their effect and where its existence was confirmed experimentally by Chambers[2].

All the material I will describe has been published, so this written version will be a summary of the talk that was given at the meeting, with references.

2. Phase monopoles

A vehicle to propel us into the unfamiliar world of wave singularities is the now-familiar geometric phase[3,4]. This phase is the flux of a 2-form in the space of Hamiltonians parameterized by $X=X_1, X_2,\ldots$. For the eigenstate $|n(X)\rangle$, the 2-form is

$$V_n(X) = \mathrm{Im}\langle \mathrm{d}n|\wedge|\mathrm{d}n\rangle \tag{1}$$

Phase monopoles are the singularities of this 2-form. They occur at parameters X^* for which the state $|n\rangle$ is degenerate. The generic case, where the degeneracy involves only two states (i.e. $|n\rangle$ and one other) and where the Hamiltonian has no symmetry, has codimension three. Thus a full exploration of the monopole singularities requires at least three parameters.

The simplest such family consists of the Hamiltonians for a spin-1/2 particle in a magnetic field $X=(X_1, X_2, X_3)$. Here the monopole[4] is at $X^*=0$. It is, however, more interesting to study the distorted monopoles in systems with more than two states. This has recently been done[5], choosing as family the *Aharonov-Bohm chaotic billiards*[6]. In these systems, a charged quantum particle moves freely in a bounded plane region D threaded by a line of magnetic flux of quantum strength α. (The purpose of the flux is to break time-reversal symmetry.) These Hamiltonians can be regarded as parameterized by the vector

$$X = \left(B_1, B_2, \alpha\right) \tag{2}$$

where B_1 and B_2 are parameters altering the shape of D. In terms of the wavefunctions

$$\psi_n(r;X) \equiv \langle r|n(X)\rangle \tag{3}$$

(depending on position r=x,y), the phase 2-form can be regarded as the vector

$$\begin{aligned} V_n(X) &= \mathrm{Im}\langle\nabla_X n|\wedge|\nabla_X n\rangle \\ &= \iint_{\text{inside D}} \mathrm{d}r\, \mathrm{Im}\, \nabla_X \psi_n^*(r;X) \wedge \nabla_X \psi_n(r;X) \end{aligned} \tag{4}$$

Degeneracies X^* can be determined by tracking the lines of V_n to their monopole sources or sinks. Several monopoles were studied in this way[5].

3. Phase dislocations

It is interesting to study the changing morphology of wavefunctions $\psi(r;X)$ in position space r, as they acquire their geometric phases during a circuit of X space. The crucial structural elements of the this process are the zeros of ψ. These are familiar as nodal lines (when r is two-dimensional) in the case where the Hamiltonian, and hence the wavefunctions, are real - because of time-reversal symmetry for example. In a study[7] of the family of triangular billiards (without flux) it was shown how in a circuit of a degeneracy (which in this case has codimension two) the nodal lines interact and change their topology so as to reverse the signs of all nodal cells and hence of ψ (for real wavefunctions the only possible phase change is π).

Things are different in the general case where there is no symmetry and the wavefunctions are complex. Then the zeros are points (in the plane), because the vanishing of a complex funtion is a codimension-two phenomenon. Writing

$$\psi \equiv \rho \exp\{i\chi\} \tag{5}$$

we see that the zeros,where the modulus ρ vanishes, are also singularities of the phase χ. In three-dimensional space these singularities are lines. We[8,9] called them phase dislocations because of a far-reaching analogy between the wavefront surfaces χ=constant (mod π) and planes of atoms in a crystal: there exist exact solutions of wave equations in which phase dislocations are of edge, screw or mixed type, can be straight or curved, can have climb or glide motion, can collide and annihilate or bounce, and can grow in loops from points (punctured wavefronts).

In Aharonov-Bohm billiards the wavefunctions possess a rich dislocation structure[10]. During a circuit near a degeneracy in X space the dislocations can change their number by collision, either with the boundary or one another[5]. In the latter case we may have either annihilation or pair production, processes obeying two topological conservation laws[11]. It frequently happens that when a dislocation is moving whilst a parameter changes, a pair is created ahead of it and one member of the pair travels back and annihilates with the original dislocation, leaving its companion moving forward; this process, analogous to the zitterbewegung of electrons, was observed previously in acoustics[12] (the parameter was time).

Most commonly, phase dislocations are free, that is, they arise by interference and are not attached to any singularity of the propagation medium; for example, the air during speech is threaded with a forest of dislocation lines. They may, however, be attached to a point singularity and be movable, but not removable, by a gauge transformation; an example is the Dirac string in the wavefunction of an electron in the presence of a magnetic monopole[13,14]. Another possibility is that they may be fixed to a physical line singularity. This occurs in the ordinary Aharonov-Bohm scattering wavefunction[1], where the dislocation is pinned to the magnetic flux line; the strength S of the dislocation, that is $1/2\pi$ times the total change in χ during a circuit of it, is the integer closest to the magnetic flux α (measured in quantum units). Therefore S changes when α passes through half-integer values, the mechanism being that wavefronts unzip all the way from the flux line to infinity and reconnect with their 2π neighbours, This interesting phenomenon cannot be observed in quantum waves (nor can S)[14], but can be and has been observed in an analogue experiment with surface ripples on water[15].

Dislocations occur on a grand scale in the tide wave[9,16,17], as 'amphidromic point' singularities of the cotidal lines (wavefronts) connecing places where the tide is high at a given time. The dislocations are therefore places of no tide (the tide is 'always high').

4. Caustics

Dislocations involve phase and so are the characteristic spatial singularities of waves. It is interesting to enquire what are the corresponding singularities in the short-wave limit, that is of classical mechanics or geometrical optics, where there is no phase. These are the caustics, that is the focal singularities of the families of rays that represent short waves. The caustic of a family is its envelope, that is the surface (in space) touched by every ray in the family. Caustics are holistic phenomena, properties of the whole family and not inherent in any one ray.

Caustics are singular because across them the number of rays passing through a point jumps (usually by two), and the ray intensity diverges: caustics are the violent births of rays. The caustics that are geometrically stable can be classified according to their codimension by the Thom-Arnold theory of catastrophes[9,18,19]. The classification is more than geometric, because to each catastrophe singularity is associated a characteristic diffraction pattern that decorates the caustic when the wavelength is small but not zero.

In the fine detail of these wave patterns, dislocations reappear as the most delicate features[9]. Sometimes the association is amazingly complicated (although stable): in the elliptic umbilic diffraction catastrophe[20], for example, there are rows of dislocation rings; in the M'th row, the number of rings is Int[512M/27 - 539/104].

As singularities, ray caustics are complementary to phase dislocations, in the sense of Bohr. The complementarity is more than the fact that caustics are infinite in intensity (in the limit of zero wavelength), whereas disclocations have zero intensity. When the wavelength is so short that a caustic emerges sharply as a singularity, dislocation singularities are lost in fine detail and cannot be resolved; and under a magnification high enough to discern the structure of an individual dislocation, the caustic singularity is smoothed away.

5. Stokes sets

It is true that in the sense just described caustics are the violent births of rays. But in another sense they are not births but really transmutations, of a complex ray into (typically) two real rays. (This is most familiar in the stationary-phase approximation of diffraction integrals, when the change of a parameter causes two complex stationary points - only one of which contributes to the integral - to coalesce and separate into two real stationary points.) One can follow the complex ray and discover the moment and manner of its birth. In contrast to what happens at caustics, this is birth is a very gentle affair, known as *Stokes' phenomenon*.

Stokes discovered[21] (in the context of the asymptotics of certain Bessel functions in the complex plane) that the birth occurs when the complex ray is at its weakest in relation to another (real or complex) ray that dominates it. If the exponentials associated with the two rays are

$$\exp\left\{k\,\phi_+(X)\right\}\ \text{(dominant) and } \exp\left\{k\,\phi_-(X)\right\}\ \text{(subdominant)} \quad \text{where } \mathrm{Re}\left(\phi_+\right) > \mathrm{Re}\left(\phi_-\right) \tag{6}$$

in which k is a (large) asymptotic quantity and X are parameters, then the maximum disparity between the exponentials, and therefore the birth, occurs when X is on the Stokes set

$$\mathrm{Im}\left\{\phi_+(X) - \phi_-(X)\right\} = 0 \tag{7}$$

Stokes sets are familiar as lines in the complex plane (arising for example in the WKB approximation of functions defined by differential equations), but in diffraction catastrophes they can occur in real parameter spaces[22,23].

Recently[24,25], the details of the birth have been determined.The birth - that is, the change in the coefficient of the subdominant wave - is governed according to a universal scenario by the error function:

$$\begin{pmatrix}\text{change in}\\ \text{subdominant cofficient}\end{pmatrix}=\begin{pmatrix}\text{dominant}\\ \text{coefficient}\end{pmatrix}\times\frac{i}{\sqrt{\pi}}\int_{-\infty}^{\sigma(X;k)}\mathrm{d}t\exp\left\{-t^2\right\}$$
$$\text{where }\sigma=\sqrt{\frac{k}{2\,\mathrm{Re}\left\{\phi_+-\phi_-\right\}}}\times\mathrm{Im}\left\{\phi_+-\phi_-\right\} \quad (8)$$

This result has generated some interest among mathmaticians[26,27,28], and applications to reflections[29] and quantum transition histories[30].

6. Complex degeneracies

For these final singularities I return to quantum adiabatics, and consider not the phase acquired by the original state during a slow parameter cycle but the probability of transition to a different state. It suffices to consider the simple 2-state Hamiltonian

$$\hat{H}\left(X(\delta t)\right)=X(\delta t)\cdot S \quad (9)$$

where $X=(X_1, X_2, X_3)$ are the parameters, S the vector of Pauli spin matrices and δ the (small) adiabatic parameter. If $\tau\equiv\delta t$ denotes 'slow time', then the history of any quantum state depends only on the *Hamiltonian curve* $X(\tau)$. We assume that there are no real degeneracies, i.e. that $X\equiv|X|$ does not vanish for any real τ, and that $X(\tau)$ is analytic in a sufficiently wide strip including the whole real τ axis. Then the probability of making a transition over infinite time is exponentially small in δ and dominated[31,32] by the *complex degeneracy* τ_c that is closest to the real axis. The degeneracy is a branch point singularity of the spectrum, determined by

$$X\left(\tau_c\right)=\sqrt{X_1^{\,2}+X_2^{\,2}+X_3^{\,2}}=0 \quad (10)$$

I report two new results related to the complex degeneracies.

The first[33] concerns the final (infinite-time) transition probability. Of course this is dominated by the familiar 'dynamical' exponential whose exponent is is proportional to $1/\delta$. But in general there is another contribution which is purely geometric in that it is independent of δ (and $\hbar$) and depends only on the geometry of the Hamiltonian curve, analytically continued from the real axis to τ_c. The reason this geometric amplitude was not noticed before is probably that it vanishes for plane Hamiltonian curves (such as that for the familiar Landau-Zener problem) and for curves that up to a rotation are identical with their time-reverse (such a uniform helix). The simplest Hamiltonian curve giving a non-zero geometric amplitude is a helix that winds from $\tau=-\infty$ to $\tau=0$ and unwinds from $\tau=0$ to $\tau=+\infty$. It would be possible to measure the new amplitude in a spin experiment involving, say, neutrons in a magnetic field.

The second result[30] concerns the transition history, that is the manner in which the final exponentially small transition probability is reached. Of course this depends on the basis states with respect to which the evolving state is described. The usual choice is the 'adiabatic basis' of eigenstates of the instantaneous Hamiltonian. In this basis, the transition takes place via rapid system-dependent oscillations of order δ, i.e. far larger than the final probability. However, there exists a series of transformations to 'superadiabatic bases', close to the adiabatic basis, for which the transition history remormalizes onto a universal one in which the increase of the transition probability is maximally smooth and compact. The transition takes place according to an error function (analogous to (8)) near the instant when the complex Stokes line emanating from τ_c crosses the real τ axis. It is possible to define spin observables corresponding to the superadiabatic bases, so that in principle the universal transition history could be observed.

7. Conclusions

I have described a cycle in the space of singularities, with each singularity being related to the previous one(s) and with the end of the cycle being not quite the same as the beginning, as is familiar in situations of this type. Here is an outline of the connections. The first singularity, inhabiting parameter space, is the phase monopole associated with an eigenvalue degeneracy. Phase dislocations - the second class of singularity - provide the mechanism for wavefunctions in configuration space to acquire their geometric phases. Caustics - the third class - are the complementary ray singularities, the loci of violent births of real rays. Stokes sets - the fourth class - are the loci of the gentle births of complex rays, of small exponentials coming into existence whilst hidden behind large ones. And finally, completing the cycle, are the complex degeneracies, from which emanate Stokes lines near whose intersections with the real time axis quantum transitions occur.

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9. References

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