IOP Publishing Nonlinearity

Nonlinearity **21** (2008) T19–T26 doi:10.1088/0951-7715/21/2/T02

OPEN PROBLEM

Three quantum obsessions

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Received 12 December 2007
Published 21 January 2008
Online at stacks.iop.org/Non/21/T19

Abstract
Is there a connection between the Riemann zeros and the quantum physics of classical chaos? Can the relation between spin and statistics be understood within elementary quantum mechanics? How are the phase singularities in classical optics smoothed by quantum effects?

PACS numbers: 03.65.Sq, 0.3.65.Vf, 0.5.45.Ac, 42.50.Ct

1. Introduction

There are three problems in theoretical physics to which I have returned repeatedly over several decades. Each sprang from a more general theme in my research. Some progress has been made, thanks to particularly fortunate collaborations, but none of the problems has been solved definitively.

Contributors to this series of papers celebrating *Nonlinearity*'s twentieth birthday were invited to supply their personal perspectives, and this account will be unashamedly personal. It will also be informal and discursive; technical details can be found in the papers cited.

1.1. Zeta and quantum

Why should a physicist be concerned with the zeros of the Riemann zeta function $\zeta(s)$, and in particular the Riemann hypothesis [1], according to which all complex zeros of $\zeta(s)$ have $\mathrm{Re}\, s = 1/2$? Not for the reasons that motivate mathematicians—fluctuations in the distribution of primes, the number of lattice points inside circles or any of the many problems to which the Riemann hypothesis is equivalent. Rather, my interest grew from research in *quantum chaology*, beginning in the late 1970s. This subject [2, 3] is the study of quantum systems whose classical counterparts possess chaotic trajectories.

Each such system has its individual spectrum of energy levels (eigenvalues of the Hamiltonian operator). However, as was clear by the mid-1980s, the statistics of the levels fall into a small number of universality classes, depending only on certain overall symmetries. The statistics are those of ensembles of random matrices. Random-matrix theory [4] had been developed earlier, to describe large data sets of energy levels in nuclear physics; the rationale was that atomic nuclei are complicated many-body systems, whose Hamiltonians might therefore be mimicked by matrices with random elements. It was natural to extend the idea to systems with few freedoms (which are therefore not structurally complicated), but whose classical motion is unpredictable—that is, systems exhibiting deterministic chaos. Numerical calculations [5–7] supported this guess, but it lacked a theoretical explanation.

In early 1985, I was developing the theory that the random-matrix universality in quantum chaotic systems was a consequence of a similar universality that had recently been discovered by Hannay and Ozorio de Almeida [8] in the distribution of long periodic orbits of the classical motion. This feature of the periodic orbits was combined with a formula relating periodic orbits to the counting function (staircase) of energy levels, due to Gutzwiller [9, 10]—a semiclassical generalization of the exact Selberg trace formula [11] for the Laplace–Beltrami operator on surfaces of constant negative curvature. Thus it was possible [12] to obtain some of the formulae of random-matrix theory. Although the physics was clear, some of the arguments involved leaps of faith. Now, better-founded arguments have been devised [13–18], and the theory is almost complete.

At the same time, I read a review paper [19], in which the heights t_n of the Riemann zeros $1/2 + it_n$ were cited as an example of numbers that are not obviously eigenvalues but which nevertheless appeared to be distributed according to random-matrix theory. This had earlier been conjectured by Montgomery [20], who noted that a formula for the correlation function of the Riemann zeros was identical to its counterpart in random-matrix theory. The tentative connection with spectra recalled an old idea, attributed [1] to Hilbert and Polya, that the Riemann hypothesis would be proved if the t_n could be shown to be eigenvalues of a self-adjoint operator.

Combining these developments, I wondered if the t_n could be the eigenvalues not of a random matrix but of a deterministic quantum system with a chaotic classical counterpart. Two observations enabled this suggestion to be converted into a testable theory. The first was the von Mangoldt formula for $\log \zeta(s)$, which when interpreted in terms of fluctuations in the counting function of the zeros took a form closely analogous to the Gutzwiller's semiclassical formula for the counting function of energy levels in quantum mechanics. By taking the analogy seriously [21], several features of the unknown dynamical system underlying the zeros could be identified, including the following: primitive periodic orbits are labelled by primes p, and their repetitions by an integer m; the period of the orbit labelled p, m is $m \log p$; the dynamical system is chaotic; all periodic orbits are unstable, with the same instability exponent; the dynamical system does not possess time-reversal symmetry.

The second observation was that in the semiclassical theory the orbit with period T describes spectral fluctuations on an energy scale $\Delta E = \hbar/T$, where $\hbar$ is Planck's constant. Therefore the long orbits, which display universality, describe spectral fluctuations and correlations of nearby levels, for which random-matrix theory holds. But the random-matrix description cannot hold for the long-range spectral fluctuations; these cannot be universal, because they are described by short classical periodic orbits, which are different from system to system. In particular, there is a shortest periodic orbit, so there is a maximum scale ΔE of spectral fluctuations.

Thus it was possible to derive explicit formulae [12] for the pair correlation and related statistics of the high Riemann zeros, in particular the number variance $\sigma^2(L)$; this is the mean-square deviation from L of the number of zeros in intervals Δt (on the critical line $\mathrm{Re}\, s = 1/2$) that contain L zeros on average. This reproduces the random-matrix formula for small L, but oscillates about a finite saturation value for large L, in a way that depends on the primes. Coincidentally, Odlyzko [22] had just performed heroic computations of many millions of high-lying Riemann zeros (near the 10^{12}th zero and near the 10^{20}th zero), with the aim of testing random-matrix theory as a quantitative description of their statistics. He had noted small deviations of $\sigma^2(L)$ from the random-matrix prediction for increasing L. Odlyzko's data provided an ideal numerical laboratory for testing the formula derived from quantum chaology, in particular the predicted deviations from random-matrix theory for large L.

The comparison, published in this journal [23], confirmed every detail of the quantum formula, including L values far beyond the random-matrix regime. The only discrepancies were some small rapid oscillations on the scale $\Delta L = 1$. At the time, I ungenerously attributed these to an error in Odlyzko's numerics, but the error was mine: Bogomolny and Keating [14, 24, 25] were able to explain the fast oscillations using more refined semiclassical arguments. The success of these predictions of deviations from random-matrix theory strongly suggests that the Riemann zeros are indeed eigenvalues of a deterministic chaotic dynamical system, and provided several clues to the nature of the system. For a review of these developments, see [26].

The pressing question is: what is the system responsible for the success of these predictions? If we knew, we would have a proof of the Riemann hypothesis. But we do not know. However, a collaboration with Jonathan Keating [27] gives a clue. From formal arguments and analogies, at the classical, semiclassical and quantum levels, it seems the dynamical system we seek could involve the following simple Hamiltonian, with a single coordinate x and its corresponding momentum p:

$$H = xp. \tag{1}$$

This has an unstable fixed point at the origin, and is not symmetric under time reversal. However, it is not bounded, and its quantum counterpart (obtained by symmetrization) does not seem to possess a discrete spectrum. What is missing is knowledge of the space on which H acts, possibly including a way to compactify the phase plane (for example by reinjecting into large p the orbits that have reached large x). Arithmetic ideas of Alain Connes [28] might lead to the answer.

One possibility is suggested by a discrepancy in the analogy between $\log \zeta(s)$ and quantum chaology: the periodic orbits contribute to the spectral counting function with the wrong sign. This was noticed long ago [21], and led Connes to propose that the Riemann zeros are not eigenvalues but points in a continuum of energy levels for which eigenfunctions cannot be defined, that is, gaps in the spectrum. A formal expression for quantum eigenfunctions incorporating the symmetries of (1) (equation (32) of [27]) indeed fails at the Riemann zeros, supporting Connes' proposal. In a sense this would be a disappointing conclusion, because it would give no evidence for the truth of the Riemann hypothesis: even for a Hermitian operator, there is no reason for non-eigenvalues to lie on the real axis. If Connes is right, (1) would be another Riemann-related system that does not lead to a proof of the Riemann hypothesis, like that of Faddeev and Pavlov [29] (see also [30]), who discovered a dynamical system (involving the Laplace–Beltrami operator on a leaky surface of constant negative curvature) for which the Riemann zeros are scattering resonances.

If there is a classical dynamical system generating the Riemann zeros as eigenvalues, it is likely to be subtle, but with hindsight it would probably be simple. The system would be an exactly solvable model for quantum chaology, analogous to the harmonic oscillator widely employed to model non-chaotic systems. Suppose that the system turns out to involve (1), as we suspect. Then since a simple rotation transforms H into $p^2 - x^2$, which is the harmonic oscillator with its potential upturned, such identification would constitute a wonderful duality, unifying the simplest chaotic system with the simplest non-chaotic one.

2. Quantum identicalness

I would have called this section 'Quantum identity', but through a quirk of the English language 'identity' is precisely the attribute that identical particles do not possess, and I wanted to avoid the ugly word 'indistinguishability'.

The spin–statistics relation is a marvellous principle in the quantum physics of identical particles. It states that under exchange of two particles (or an odd permutation of N particles) the quantum state acquires a sign $(-1)^{2S}$, where S is the spin (integer for bosons, half-odd-integer for fermions). For electrons, spin–statistics is the Pauli exclusion principle, underlying the periodic table of the chemical elements and the impenetrability of condensed matter made of atoms that are mostly empty. For bosons, it is responsible for the operation of lasers, and is fundamental in the explanation of superconductivity and superfluidity. Clearly, the spin–statistics relation is a mighty fact about the world.

Where does the principle come from? The common view is that in ordinary quantum mechanics it is a separate postulate, whose derivation as a theorem requires relativistic quantum field theory. The theorem has been developed at different levels of sophistication and under an evolving set of assumptions, starting with work by Pauli [31]; a detailed and scholarly review is provided by Duck and Sudarshan [32], who question the relativity requirement but insist on quantum field theory [33].

However, there have been persisting suspicions that spin–statistics might somehow be contained in the ordinary non-relativistic quantum mechanics of finitely many identical particles. In particular, Feynman [34] was unhappy that a principle which could be stated so simply required such a sophisticated derivation. I shared this dissatisfaction, and in the early 1980s my attempts to find an elementary derivation were focused by the development of *geometric phases* as a theme in my research.

The thought that spin–statistics has a geometric origin was strengthened by familiar conjuring tricks with twisted ribbons; this invocation of a macrosopic analogue was most clearly described by Hartung [35], and is beautiful enough to bear repeating. The argument, intended to explain the sign change for fermions, can be summarized in two steps, as follows. First, imagine the two fermions connected by a ribbon, with one held in each hand. Cross the hands, so as to exchange the fermions without rotating them. Then the ribbon, whose role is to keep track of the exchange, develops a twist, which can be undone by rotating either of the particles (ends of the ribbon) by 2π. There are several similar tricks, all illustrating the fact that every exchange involves a hidden rotation. In effect, this reduces the two-body problem of explaining the sign change under exchange to the one-body problem of understanding the sign change under rotation of a single fermion.

Second, with one end of the ribbon fixed, twist the other (representing a fermion) by two complete turns (4π). It is possible to manoeuvre the fixed end, without rotating it, so as to undo the twist. This is not possible with one turn. The conclusion is that two turns are equivalent to no turns but one turn is not. At the microscopic level, this property of turns in space (double covering of the rotation group in three dimensions) corresponds to a sign change of spinors on rotation, and so, by the equivalence described in the previous paragraph, to a sign change under exchange.

This suggestive argument is a good way to describe unexpected implications of geometry to people who are not scientists. But of course it is very far from a convincing quantum-mechanical argument. Over several years, I sought to explain spin–statistics by incorporating time-dependent parameters in the Hamiltonian for the two spinning particles, to forcibly interchange the particles adiabatically, in the hope that $(-1)^{2S}$ would emerge as a geometric phase. These attempts failed.

In fact the emergence of spin–statistics from elementary quantum mechanics requires a quite different approach, developed in collaboration with Jonathan Robbins in the early 1990s [36, 37], in which indistinguishability is incorporated into the Hilbert space of two- (or $N-$) particle states. For two particles, this requires identification of positions $\{\boldsymbol{r}_1, \boldsymbol{r}_2\}$ with $\{\boldsymbol{r}_2, \boldsymbol{r}_1\}$ in the six-dimensional configuration space. This approach had been pioneered by Laidlaw and DeWitt [38] and Leinaas and Myrheim [39] for particles without spin. For spinning particles, identification of positions requires states to be represented in an unusual basis, in which the spins are not specified in a fixed basis (e.g. by their z components) but are linked to positions in such a way that exchange of positions smoothly exchanges the spin states. Only with this 'transported basis' is indistinguishability incorporated completely. Then it is possible to insist that the wavefunction is single-valued in this new space with exchanged positions identified. The appeal of single-valuedness is that it makes exchange of identical particles similar to other quantum operations that leave the physics unchanged.

Constructing the transported basis required some technicalities. We found it convenient to use Schwinger's representation of each spin in terms of two harmonic oscillators [40]. Transforming back to the usual fixed basis, $(-1)^{2S}$ emerged automatically. The corresponding phase $2S\pi$ is associated with a non-contractible circuit, representing exchange, in the projective plane corresponding to the direction of the interparticle unit vector $(\boldsymbol{r}_2 - \boldsymbol{r}_1)/|\boldsymbol{r}_2 - \boldsymbol{r}_1|$ with antipodal points identified. Therefore the spin–statistics sign can be interpreted as a topological phase with the fixed value $2S\pi$, rather than the usual geometric phase which can vary continuously because the corresponding circuits can be continuously shrunk to zero. This topological phase was not unanticipated; an example had been identified in the m=0 subspace for a single spin in an adiabatically varying magnetic field [41].

This was a gratifying outcome, but is it a proof? Unfortunately not, because the transported basis we constructed is not the only possible one, and some alternative constructions [42] give the wrong spin–statistics connection. However, subsequent work by Jonathan Harrison and Robbins [43,44] indicates that there is a group-theoretic sense in which the original transported basis [36] is the simplest one. It remains to be seen whether our approach, incorporating indistinguishability into the Hilbert space and then invoking single-valuedness, gives lasting insight into the spin–statistics connection.

Arising from this research is a moral for society's support of fundamental science. In the early 1990s, we applied for funding from two sources, to support Robbins in the initial stages of our collaboration. Both applications were successful, with the (presumably different) referees encouraging the project but doubting that our approach could succeed. And indeed after two years we had to confess to the supporting agencies that our attempts to understand spin–statistics had failed (but that we had put their funds to good use in other research). However, several years later Robbins realized that the work we had done was in fact not futile, and we returned to the subject, with the results described above. This illustrates the folly of assessing the outcome of funded research on a short-term basis.

3. Quantum blurring of classical optical singularities

This arose from my research on *asymptotics* and *singularities of waves*. In the 1960s, I realized that in the short-wave limit the significant features of coherent wavefields, where waves are most intense, are the caustics underlying the wave; caustics are the envelopes of the family of geometrical rays or classical paths. Precisely at these most important places, the simplest geometrical asymptotics (WKB for differential equations governing the waves, stationary phase for their integral representations) break down. More sophisticated asymptotics [45–47], later incorporating the classification of caustics by catastrophe theory [48,49], is required to describe how the geometrical singularities are softened by diffraction.

The passage from rays to waves, in which the singularities disappear, introduces a new concept: phase. In the 1970s, John Nye and I [50, 51] realized that phase has its own singularities: places where the wave amplitude is zero. In a sense, phase singularities (also called optical vortices or, in three dimensions, wavefront dislocation lines or nodal lines) are complementary singularities to caustics [52].

This phenomenon, of the singularities at one level of theory being dissolved at the next, is more general. In classical optics, for example, the next level of approximation beyond scalar waves is the vector (Maxwell electromagnetic) description. In vector waves, phase singularities disappear (the codimension is too great for them to be stable). But the passage from scalar to vector waves introduces a new concept: polarization. And in the 1980s Nye, in collaboration with Hajnal [51,53] realized that polarization possesses its own singularities, namely, lines in space where the polarization of the light is purely circular or purely linear.

Already in the mid-1970s, before polarization singularities were discovered, I imagined that this process of progressively dissolving singularities would persist at the more fundamental level of the transition between (scalar) wave optics to quantum optics. The idea was that the dark light of a phase singularity would be faintly illuminated by the glimmering of the quantum vacuum. I struggled to make a precise prediction of the way in which vacuum fluctuations would soften the phase singularity, but was frustrated by my lack of expertise in quantum optics.

But a few years ago, in collaboration with Mark Dennis, this idea bore fruit. We imagined a classical light wave, that is an optical mode containing many photons, with a phase singularity, all other modes being in their vacuum states. To explore this mode, we envisaged an excited atom and calculated the intensity of its decay as a function of position. Far from the singularity, the decay would be dominated by stimulated emission [54] from the classical wave. Close to the singularity, where the classical wave is weak, the intensity would be dominated by spontaneous emission into the unoccupied vacuum modes.

In particular, we calculated [55] the radius of the quantum core, within which spontaneous emission dominates:

$$R_{\mathrm{Q}} \approx \sqrt{\frac{\hbar\omega^3\Delta\omega}{2\pi^2c^3C}}. \tag{2}$$

In this formula, Planck's constant $\hbar$ enters because the core is a quantum effect, ω is the frequency of the light, $\Delta\omega$ is the line-width of the detecting atom and $C = |\nabla\psi|^2$ describes the linear local neighbourhood of the phase singularity. For a 5 mW helium–neon laser in a Laguerre–Gauss mode with a first-order phase axial singularity, focused to a waist width 100 μm, detected by a hydrogenic atom ($\Delta\omega \sim 5 \times 10^6\,\mathrm{s}^{-1}$), the formula gives $R_{\mathrm{Q}} = 1\,\mu$m. This should be detectable, and we hope that the experiment will be performed, perhaps with an atom trapped in a cavity containing the singular field.

Theoretically, the core is a fundamental quantum-optics effect, combining three types of singularity: the phase singularity that is being smoothed, the singular semiclassical (small $\hbar$) limit in which the core emerges as a distinct structure and the spectral singularity associated with the degeneracy (or near-degeneracy) of the unoccupied modes into which the detecting atom can decay spontaneously. Nevertheless, there is a sense in which the result is disappointing, because the quantum smoothing of a classical-optics singularity appears to possess far less richness than, say, the diffraction catastrophe smoothing of geometrical caustics. The core underlying (2) merely reflects the inert addition of a locally constant vacuum term to the classical intensity. It is possible that there are richer core effects for higher field correlations or associated with quantum smoothing of classical polarization singularities.

Analogous effects should occur for other types of wave. In sound, for example, phase singularities are fleeting threads of silence. But in their quiet centres the silence is destroyed by the whispering associated with pressure fluctuations of the gas molecules—fluctuations analogous to chaos of the quantum vacuum, and audible in principle as Brownian fluctuations on a detector. For the human eardrum, such fluctuations are just below the detection limit (there seems no useful purpose in hearing Brownian motion), but calculations [55] indicate that the acoustic cores could be revealed by a more sensitive broadband detector.

Acknowledgments

My research over many years has been supported by the Royal Society and the University of Bristol.

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