QUANTUM MECHANICS, CHAOS AND THE RIEMANN ZEROS
(Closing talk)

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With some meetings it would be appropriate for the closing speaker to summarise the talks. I think that is impossible here because the contributions have been too diverse, and in any case I did not understand all of them. Any summary would reflect only my prejudices and would add nothing. So I said to Yakov Shnir if I could use these closing remarks to present some physics, and he kindly agreed.

What I am going to do, without technicalities - that is, with voice and hands - is describe an area of quantum physics that has not been represented in this meeting, namely the quantum mechanics of systems whose classical trajectories are chaotic. In these systems, all trajectories are unstable: they diverge exponentially from the neighbors. This is a problem that has achieved much attention in recent years - in the last twenty years - and it is interesting,important, and, for several reasons, fundamental.

First, we really ought to know after so many decades what the relation between quantum mechanics and classical mechanics, when the classical motion is chaotic. This problem falls outside the class of usual asymptotic methods. For example, the adiabatic method, which was described in one of the talks here, and which goes back to 1911, does not work when there is chaos. All generalizations of Bohr-Sommerfeld, for example by Einstein, by Wentzel-Kramers-Brillouin, and by Keller and Maslov - all these depend on the existence of action-angle variables, and such variables do not exist for chaotic motion. This is one reason.

Another reason is that we now begin to see experiments of this area. Some involve hydrogen-like atoms in a very strong magnetic field; in this case the competition between the Kepler ellipses you would get with Coulomb field alone, that is without magnetic field, and the the Larmor helices you would get with the magnetic field alone, that is without the Coulomb field, gives chaos. Again with highly excited vibration-rotation states of complicated molecules one has essentially nonlinear springs and large regions of chaotic motion in the phase space which are associated with many if not most of the quantum energy levels. Experiment can measure hundreds - sometimes thousands - of such levels, and it is important to understand what determines these levels, that is what determines quantization. Of course the Schrödinger equation determines quantization but for higher excited states - especially in these chaotic systems- numerical methods get ever more difficult. One can carry them out but one gets little inside from them into the origin of quantization and the relation with classical chaos.

What I am going to tell you in these few words is that there is a deep and beautiful relation, still mysterious, between this problem of chaos and quantum mechanics and the Riemann ζ-function of number theory. It involves the prime numbers in an essential way. It is a very satisfying thing to begin to see in physics an applications of prime numbers. Almost every piece of mathematics that has strength and depth appears in physics sooner or later; in recent years we come to learn this more and more. Prime numbers, which are the atoms of arithmetic, have not so far been applied. Of course integers have - indeed the very beginnings of our subject of mathematical physics concern with Pythagoras' observation that the lengths of vibrating strings which sound harmonious are in integer ratios. Integers, yes, but primes, not.

Let me explain the physical problem that the Riemann ζ-function helps us to solve. It is not true that we have no theory for chaotic quantum systems. We do have the theory. It is based on the following idea. Consider the spectral density (the density of states). This is a series of delta-functions, one for each energy level (we consider only bound systems). The crudest and simplest question one can ask is: What is the average density of such states? What is the smoothed density? The answer is given by a very old formula brought to perfection by Herman Weyl. The Weyl formula is based on the idea which we all khow as physicists, that roughly speaking is the phase space of a system with d freedoms each quantum state corresponds to a volume $\hbar^d$. This idea gives very quickly an approximate but rather accurate formula for the smoothed level density.

Of course, all the interesting problems, and in particular the difference between a system which is chaotic and one which is not, lie beyond the smooththed spectrum. One must consider fluctuations. For this we have a beautiful theory. It is due to Gutzwiller and Balian and Bloch. The theory says that to the smooth background which gives the average level density there must be added oscillations. It is a bit like a Fourier series. More and more oscillations can be added and the hope is that they conspire by constructive interference to give the delta spikes of the spectrum. The central point is that each oscillation is associated with a periodic trajectory of the classical motion.

It is commonly believed, but generally false, that each periodic trajectory determines by itself a family of levels. This is true only in special cases, for example for some states of a system with a stable periodic trajectory. In chaotic systems there are no stable orbits and the one-to-one association is wrong. What is right is that each periodic trajectory determines an oscillatory contribution to the spectrum density. The longer the orbit (and therefore the more complicated) the more rapid is the oscillation it contributes.

So there is a relation of mutual collectivity between the set of all periodic trajectories and the set of all levels. This is the Gutzwiller formula. In some special cases it is known to mathematicians as the Selberg trace formula. It is extremely useful in a large class of problems if one does not wish to find the position of each individual level, but rather a rough picture of the clustering of levels on scales large compared with the level spacing. For example there is great potential for applying the formula in acoustics. The idea here is that these quantum problems are isomorphic to other wave problems, for example waves in two- or three-dimensional enclosures like this room. In the case where the geodesic motion is nonintegrable one has the class of 'quantum chaology' problems I am interested in. If one wants the spectrum with its finest details - that is the individual levels - smoothed away, Gutzwiller's formula in its native form is very useful.

However if one wishes to make serious use of it to sum all periodic trajectories and see the emergence of the individual levels as spikes, it fails completely. The reason it fails is that it does not converge in any meaningful sense. Why? The reason is that in a chaotic system there is an enormous number of periodic trajectories. The number of periodic trajectories with period less than T grows as $e^{\lambda T}$, where λ is the entropy which measures the chaos. So the periodic trajectories proliferate exponentially and ruin meaningful calculation with the Gutzwiller sum.

This is the place where the Riemann ζ-function enters the story. You probably know that it is a function of complex variable z. It is the sum of inverse powers of integers or, more relevantly, a product over primes:

$$\zeta(z) = \sum_{n=1}^{\infty} \frac{1}{n^z} = \prod_{primes\ p} \frac{1}{1 - p^{-z}}$$

This is the intimate relation between the ζ-function and the primes. The celebrated Riemann hypothesis is the conjecture that the compex zeros of $\zeta(z)$ lie on the line Re z = 1/2 (where the above formulae do not converge and must be interpreted by analytic continuation). The relevance of this function to our physical problem lies in the fact that much evidence tells us that the Riemann zeros are distributed exactly like the energy levels we are trying to understand, of quantum systems that are classically chaotic. So an understanding of Riemann zeros can help us understand a quantum problem, and quantum mechanics can tell us new things about the Riemann ζ-function.

What the basis of this unbelievable assertion? It comes from an expansion of the logarithm of $\zeta(z)$, whose derivative is related to the density of Riemann zeros. One can express this as a smooth part, which is understood, and oscillations. The oscillations have almost exactly the same form as those in Gutzwiller's formula. Therefore it is natural to identify them with the periodic orbits of something. This leads to a very useful analogy. The basis is the idea that the Riemann zeros (rotated by 90°) are eigenvalues of something. This is an old idea, going back nearly a century. If the 'something' were a self-adjoint matrix, then the eigenvalues would be real and this would prove the Riemann hypothesis. We do not know what the operator is. However there is good reason to conjecture that it is not just any self-adjoint operator but one with a classical limit, namely some dynamical system. We know much about this system, even though we cannot identify it. Here are some of its properties:

1. The trajectories are chaotic, with entropy unity for all trajectories.
2. The dynamical system does not have time-reversal symmetry - rather like a particle in a magnetic field which does not retrace its steps if the velocity is reversed.
3. Most importamt, the periodic orbits have periods which are multiplies of logarithms of prime numbers.

This still seems an unlikely and possibly superficial analogy. I want to convince you that it is not, by telling you how the analogy was first used, and then I will tell you how we are using it now. It was first used to learn about the statistics of the Riemann zeros.

Looking high in a quantum spectrum, it is natural to ask about the statistics of the levels. The simplest statistic is the mean level density, which is trivial. More interesting are the fluctuation statistics. One such is the number variance, defined as follows. Choose a range where on the basis of the mean level density we would expect L levels - the average number in the interval. Of course the actual number N will fluctuate about L and it is natural to enquire about its variance $< (N-L)^2 >$, where the average is over some range of energy. The number variance depends on L and so can describe both short and long range spectral correlations. This statistic can be calculated using the Gutzwiller formula along with two rather nontrivial additional ideas, giving an expression which does converge. For small L the variance is dominated by long orbits, since by Heisenberg's principle the period corresponding to a range of δE is $\frac{T=\hbar}{\delta E}$. The smaller the range, the larger the relevant classical periods. In this range (small L) the statistics are universal, that is, the same for all chaotic systems (apart from some refinements involving symmetry). This spectral universality comes from a classical universality: all very long classical trajectories are, in a sense, the same, in that they cover the energy surface uniformly after slight coarse-graining. But for larger L, corresponding to longer energy ranges, the relevant orbits are shorter, and the number variance begins to discriminate between one chaotic system and another and so becomes nonuniversal. Eventually, when L is large enough, there are no shorter periodic orbits and the fluctuations saturate.

This theory can be applied to $\zeta(z)$, that is, quantum mechanics can be applied to arithmetic. I did this some years ago. I was fortunate to have access to a wonderful numerical laboratory of Riemann zeros computed by Andrew Odlyzko. He computed 200 000 000 Riemann zeros starting at the 10^{20} - undoubtedly asymptotic. Those calculations took 1000 hours of Cray time and 2000 MB of store. With the 'semiclassical' theory, involving periodic orbits and hence primes we know every term in the analogy and the calculations of the Riemann number variance can be made in a few seconds on a personal computer. The result was that the theory reproduces every little detail of the number variance calculated by Odlyzko, in both the universal and nonuniversal regimes.

So quantum mechanics applied to $\zeta(z)$ was able to tell mathematicians something rather refined and new about the Riemann zeros. This gave confidence in the value of the analogy, justifying proceeding further and trying to use the analogy to calculate individual levels instead of just statistics. This is the 'holy grail' of quantum chaosology: the calculation of individual levels. As I have said, Gutzwiller's formula fails for this. It fails in a deep way, that reflects an important fact about quantum and classical mechanics: the limit of small $\hbar$ - the semiclassical limit - does not commute with the limit of long times. Given an evolving state, represented by a wavepacket, then under semiclassical conditions the evolution can be well approximated by the elementary semiclassical propagator for some time. But after a long time (in order $\hbar$ divided by the mean level spacing and so classically long for more than one freedom) the system starts to evolve differently from its classical counterpart. Quantum motion is always multiply periodic because the spectrum is discrete, whereas classical chaotic motion has a continuous spectrum and so is periodic. After a long time, that difference becomes apparent. This is absolutely fundamental, and we study spectra because these involve the energies of stationary states - stayes that do not change with time - so we are forced to confront head on the long-time, small-$\hbar$ clash.

As you might guess from the fact that Odlyzko was able to calculate so many Riemann zeros, there are better ways of calculating those zeros than calculating quantum levels, which we quantum physicists might benefit from learning. So, what do the mathematicians do? They do not calculate the density of zeros. There is a slight modification of the $\zeta(z)$ which is real where the zeros are and this is whatis calculated. The simplest scheme would be to use the simple Dirichlet series writen above, but this does not converge. What mathematicians do is use a formula discovered by Riemann which remained hidden until Siegel found it sixty years later. The extremely powerful Riemann-Siegel formula is based on the following idea. Take the Dirichlet series, truncate it at the term whose phase is stationary (this varies with the height of the zero, that is with what we call energy), and then resum the divergent tail. Now comes an example of a beatiful phenomenon that has been explored a lot in recent years, an idea from asymptotic with wide applications. Very often the resummation of high orders of a divergent series gives contributions related to the low orders of another series, or even the same series. In this case it is the same series. So the high integers (related to the high primes) fold back and give contribution complementary to the low integers. This leads to a compact formula for $\zeta(z)$, plus corrections.

It is natural to try to apply a 'Riemann-Siegel looklike' formula to quantum mechanics. This possible only to leading order, and is not very accurate. The Riemann-Siegel corrections are hard to interpret in mechanics. Jonathan Keating and I decided to use the intuition behind the Riemann-Siegel formula to derive an improved version of it, which can be applied - corrections included - to quantum mechanics. If the formula is applied to $\zeta(z)$ it easily yields accuracy much greater than Riemann-Siegel with comparable effort (10^7 times better in a typical case).

When applied to quantum mechanics, the new formula amounts to analytic continuation with respect to $\frac{1}{\hbar}$, from a region of $\frac{1}{\hbar}$ where the Gutzwiller series converges. This region has a finite imaginary part. The resulting version of Gutzwiller's formula (rather its exponential, representing the spectral determinant) is free of divergence. Recently Keating and Sieber have made beautiful computations testing the various formulae on the following system: billiard consist of a particle moving in the part of the plane between a right-angled corner and a hyperbola. Although the hyperbola billiard is unbounded, it does have a discrete spectrum. Much is known about the periodic trajectories. The improved Riemann-Siegel formula works wonderfully well for this system, not only for the zeros but for the whole spectral determinant as a function of energy.

Now, although this is a very satisfactory development it is not the end of the story, because when applied to quantum mechanics - as opposed to $\zeta(z)$ - the new formula, although it converges, still involves too many periodic orbits. The number that contributes increases much too fast as energy increases. This is bad because in a proper semiclassical formula the calculations should either get easier for high excited states or at least get difficult more slowly than the increase in the number of levels. This is not yet the case, for a deep reason I will not go into and which we are trying to remedy.

What I have tried to tell you is that there is now this two-way traffic between unexpected branches of science: chaos and quantum mechanics, and Riemann zeros and prime numbers. Of course, the reason we physicists are interested in $\zeta(z)$ is not the same as the mathematicians' reason. They want to prove (or disprove) the Riemann hypothesis. For us this would be just a by-product. We are interested for the following reason. For nonchaotic systems we have the harmonic oscillator as the exemplar of that class. Almost everything about classically integrable systems reduced in some way, locally or globally, to some aspect of the harmonic oscillator. This is not true for chaotic systems. Now $\zeta(z)$ is in some sense a very simple function, although subtle. If the operator could be found - that is the classical dynamical system could be found of which the operator is the quantization - then this would surely be an exemplar of the class of classically chaotic quantum systems and an ideal case against which all calculations and models could be tested.

I have enjoyed this meeting very much, and so, I am sure has everybody else, in several ways. On way is scientifically. It is always exciting to meet brothers and sisters in a community with which until now we have had little contact. It is beautiful to find people interested in the same problems and studying in similar way. We are all part of the universal scientific culture which can exists even in the most disjoint communities. And of course we have enjoyed this place and the splendid organization that has been provided by the committee here and by the staff here. Abundant thanks for your hospitality and for your many kindnesses.