

INTRODUCTION TO MATHEMATICAL ASPECTS OF QUANTUM CHAOS

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Keywords: arithmetic quantum chaos, Anosov system, Berry-Tabor conjecture, Bohigas-Giannoni-Schmit conjecture, classically chaotic system, classically integrable system, geodesic flow, Hecke operator, Hecke cusp eigenfunction, holomorphic modular form, invariant tori, Kolmogorov-Sinai entropy, Laplace-Beltrami operator, L-functions, Maass wave form, microlocal lift, quantization of Hamiltonian flow, quantization of torus maps, quantum chaos, quantum ergodicity, quantum limit, quantum unique ergodicity, random matrix theory, Rudnick-Sarnak conjecture, semiclassical limit, semiclassical measure, sensitivity in initial conditions, spectral statistics, Wigner distribution, zeta functions

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Summary

This is a review of rigorous results obtained up to now in the theory of quantum chaos and also of the basic methods used thereby. This theory started from several conjectures about the way how the behavior of a quantum system is influenced by its classical limit being integrable or chaotic. Numerical calculations suggested that Wigner's statistical approach to the spectra of heavy nuclei via large random matrices seems to be applicable quite generally to quantum systems with chaotic classical limit.

On the other hand, the construction of semiclassical solutions of the stationary Schrödinger equation for quantum systems with integrable classical limit, whose generic orbits cover invariant tori in phase space, lead to the expectation, that eigenstates of classically chaotic quantum systems should, like their generic classical orbits on the energy hypersurface, be equidistributed in configuration space.

Even if progress in understanding general quantum systems rigorously is slow, there is a class of systems where important results have been obtained, namely those systems, which have nice arithmetic properties and are directly related to problems in number theory. For them the methods developed there can be applied. On the other hand, this connection influenced also research in number theory, as for instance on the statistical

properties of zeros of number theoretic functions like zeta or L -functions. This whole circle of problems is now combined under the name “arithmetic quantum chaos”, and the results there constitute the main body of this report.

Since the whole theory is still in plain development with many open problems and therefore far from being a complete theory, this chapter tries only to review and describe the current situation and has certainly to be reworked in the future.

1. Introduction

1.1. Einstein’s Quantization Rules

The origin of the theory of quantum chaos, which in the physics literature is sometimes also called ‘quantum chaology’ (Berry, 1987), is a paper by Einstein (1917), which at his time did not find much attention in the scientific community. In this paper he discussed the so called ‘old quantum mechanics’ of Bohr, Sommerfeld and Epstein and their approach to pass from classical mechanics to the quantum spectrum of a Hamiltonian system with N degrees of freedom and Hamilton function $H = H(\underline{x})$. He gave a coordinate independent formulation of Sommerfeld’s quantization rules which are valid for general completely integrable systems and not only for the separable ones among them, which can be reduced to N uncoupled systems with one degree of freedom. For such a completely integrable system with N degrees of freedom Einstein’s quantization conditions have the form

$$\oint_{\gamma_i} p \underline{d}q = n_i h, \quad n_i \in \mathbb{N}, \quad 1 \leq i \leq N, \quad (1)$$

with h Planck’s constant. The γ_i ’s denote “closed curves in q -space to which all closed curves can be reduced by continuous deformations” to use Einstein’s original formulation. In modern language, they are the N cycles determining a basis of the fundamental group of an invariant N -torus \mathbb{T}_N in the phase space $\Gamma = \{\underline{x} \in T^*(M)\}$, the cotangent bundle of configuration space M of the completely integrable system. In local canonical coordinates the so called microstates \underline{x} are then given by $\underline{x} = (\underline{q}, \underline{p}) \in \mathbb{R}^{2N}$. The main remark Einstein’s in (1917) however concerns the fact, that for systems not integrable, like for instance Poincaré’s 3-body system, this method does not work.

Einstein therefore formulates the problem, how to determine the quantum spectrum of a system whose classical limit in the extreme case has no invariant tori at all and whose generic trajectory in phase space is dense on the entire energy shell $\Gamma_E = \{\underline{x} \in \Gamma : H(\underline{x}) = E\}$. This is the case for what one calls nowadays classically chaotic systems and whose time evolution $\Phi_t^H : \Gamma_E \rightarrow \Gamma_E$ on the energy hypersurface Γ_E depends sensitively on initial conditions. This means, that the Hamiltonian flow

Φ_t^H has at least one positive Liapunov exponent $\lambda = \lim_{t \rightarrow \infty} \frac{\log((D\Phi_t^H)(\underline{v}))}{t} > 0$ for almost all $\underline{x} \in \Gamma_E$ with respect to the invariant measure on Γ_E induced from Liouville measure $d\mu_L(\underline{x}) = d\underline{q} d\underline{p}$, and some tangent vector $\underline{v} \in T_{\underline{x}}(\Gamma_E)$. On the other hand, the time evolution of a quantum system with Hamilton operator $\hat{H}_\hbar = -\frac{\hbar^2}{2m}\Delta + V(\underline{q})$, with Δ the Laplace operator in \mathbb{R}^N , which is given by the unitary operator $U_\hbar(t) = \exp\left[-\frac{i}{\hbar}\hat{H}_\hbar t\right]$ in a Hilbert space \mathcal{H} , cannot be chaotic in this sense for $\hbar \neq 0$, since it is in general quasiperiodic and hence does not depend sensitively on the initial state in \mathcal{H} . This already shows the singular character of the so called semiclassical limit $\hbar \rightarrow 0$ of quantum physics which obviously is not a small perturbation of the limit $\hbar = 0$ of classical mechanics.

1.2. The Berry-Tabor Conjecture on the Local Statistics of the Eigenvalues of Classically Integrable Systems

Numerous numerical calculations have shown that in the semiclassical limit $\hbar \rightarrow 0$ one can find nevertheless typical fingerprints of its classical limit in the spectrum of a quantum system, which depend on this classical limit being integrable or chaotic. Already from Bohr's correspondence principle one expects physically, that a quantum system with Hamilton operator $\hat{H}_\hbar = -\frac{\hbar^2}{2m}\Delta + V(\underline{q})$ should behave more or less classically when Planck's constant \hbar is "small". A typical case for instance for this is the situation, when the system's de Broglie wavelength $\lambda = \frac{\hbar}{\sqrt{2m(E-V(\underline{q}))}}$ is very small compared to the characteristic distance over which the potential V varies appreciably, the so called short wave length respectively high frequency limit.

Another example is the case of a free particle, moving in a bounded region like a billiard table, with Hamilton operator $\hat{H}_\hbar = -\frac{\hbar^2}{2m}\Delta$ with $\Delta = \partial_x^2 + \partial_y^2$ the Euclidean Laplace operator with vanishing boundary conditions, where the semiclassical limit $\hbar \rightarrow 0$ corresponds to the high energy behavior $E \rightarrow \infty$ of the quantum system.

The numerical investigations of different quantum systems resulted in a couple of conjectures both concerning properties of the eigenvalues $\lambda_i(\hbar)$ and the eigenstates $\psi_i(\hbar)$ of the Hamilton operator, given by $\hat{H}_\hbar \psi_i(\hbar) = \lambda_i(\hbar) \psi_i(\hbar)$, which indeed are the main focus of the research in quantum chaos over the last years: for the eigenvalues $\lambda_i(\hbar)$ of a quantum system whose classical limit is completely integrable, Berry and Tabor (1977) formulated the conjecture, that generically the local statistics of its appropriately rescaled eigenvalues should be Poissonian in the semiclassical limit $\hbar \rightarrow 0$. This means for instance for the consecutive level spacing distribution

$P_n(s) = \frac{1}{n} \sum_{i=1}^n \delta(s - \hat{\lambda}_{i+1} + \hat{\lambda}_i)$ of the unfolded eigenvalues $\hat{\lambda}_i$ with unit mean spacing

distance, that $\lim_{n \rightarrow \infty} P_n(s) = P(s)$ should be given by $P(s) = e^{-s}$, analogous to the waiting times between consecutive completely independent random events.

1.3. The Bohigas, Giannoni and Schmit Conjecture for the Local Statistics of the Eigenvalues of Classically Chaotic Systems

For quantum systems with chaotic classical limit on the other hand, Bohigas et al (1984) suggested in analogy to Wigner's approach to the spectra of heavy nuclei, whose classical dynamics is expected to be highly chaotic, that their rescaled spectra should follow in the semiclassical limit $\hbar \rightarrow 0$ the spectral statistics of the eigenvalues of certain Gaussian ensembles of large matrices depending on the systems invariance properties under time reversal (respectively under space rotations for systems with half-integer spins). The corresponding Gaussian measures have the form

$$d\mu_N(\hat{H}) = C_n \exp\left(-\frac{\text{trace}\hat{H}^2}{v^2}\right) d\hat{H}, \quad d\hat{H} = dH_1 \cdots dH_f, \quad (\text{where } f \text{ denotes the number of}$$

independent real variables of the matrix \hat{H}) and are supported on large real symmetric $N \times N$ matrices for systems invariant under time reversal respectively on large $N \times N$ Hermitian matrices for systems lacking time reversal invariance as for instance systems with magnetic fields. The measure $d\mu_N(\hat{H})$ on symmetric matrices is obviously invariant under conjugation of \hat{H} by orthogonal matrices, hence its name Gaussian orthogonal ensemble (GOE), whereas the measure on the Hermitian matrices is invariant under conjugation by unitary matrices, hence its name Gaussian unitary ensemble (GUE). For the common distribution $P(\lambda_1, \dots, \lambda_N)$ of the eigenvalues $\{\lambda_i\}$

one then finds $P(\lambda_1, \dots, \lambda_N) = C_{N,\beta} e^{-\sum_{i=1}^N \left(\frac{\lambda_i^2}{4v^2}\right)} \prod_{i < j} |\lambda_i - \lambda_j|^\beta$, where $\beta = 1$ for the GOE and

$\beta = 2$ for the GUE ensemble. From this one derives for large N for the consecutive level spacing of the unfolded eigenvalues to a close approximation for the GOE ensemble the so called Wigner surmise $P(s) \sim \frac{\pi}{2} s \exp(-\pi s^2 / 4)$, respectively for the GUE ensemble $P(s) \sim \frac{32s^2}{\pi^2} \exp(-4s^2 / \pi)$. Hence for chaotic systems consecutive levels of the quantum system should repel each other, whereas in the integrable limit case they should accumulate. For the level density

$$\rho_{N,\beta}(\lambda) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} P_{N,\beta}(\lambda, \lambda_2, \dots, \lambda_N) d\lambda_2 \cdots d\lambda_N$$

one gets in the large N limit independent from β

$$\begin{aligned} \rho_N(\lambda) &\sim \frac{1}{2\pi} \frac{1}{Nv^2} \sqrt{(4Nv^2 - \lambda^2)} && \text{for } |\lambda| < 2\sqrt{Nv^2} \\ &\sim 0 && \text{for } |\lambda| > 2\sqrt{Nv^2} \end{aligned}$$

For the distribution of the variable $x = \frac{\lambda}{\sqrt{Nv^2}}$ hence one gets Wigner's semicircle law

$$\rho(x) = \frac{1}{2\pi} \sqrt{4-x^2} \quad \text{for} \quad |x| < 2$$

$$= 0 \quad \text{for} \quad |x| > 2.$$

Rigorous results concerning these conjectures on the local spectral statistics of quantum systems in the semiclassical limit have been obtained up to now only for systems with nice arithmetic properties, to which methods from number theory can be applied.

1.4. Berry's Conjecture on the Equidistribution of Eigenfunctions for Classically Chaotic Systems

Another characteristic of a quantum system where possible fingerprints of its classical behavior can be found, is the morphology of its bound states in the semiclassical limit, that means the eigenfunctions of its Schrödinger operator $\hat{H}_\hbar = -\frac{\hbar^2}{2} \Delta + V(x)$, when \hbar tends to zero.

1.4.1. Arnold's Quasimodes

The reason for such an expectation can be understood when looking at systems with completely integrable classical limit. One knows from semiclassical quantum mechanics, which started for systems with one degree of freedom with the so called JWKB approximation, named after the mathematician Jeffreys and the physicists Wentzel, Kramers and Brillouin, that one can use the invariant tori of these systems to construct the so called "quasimodes" of Arnold (1972). In special cases these quasimodes turn out to be indeed approximate solutions of the stationary Schrödinger equation (Jakobson and Zelditch, 1999) with eigenvalues determined by Einstein's quantization conditions, which were later corrected by the above authors respectively Keller and especially Maslov. These corrected conditions can be shown to follow basically from single-valuedness of these quasimodes ψ which in local coordinates have the following form

$$\psi(\underline{q}) = \sum_l A_l(\underline{q}) \exp\left(\frac{i}{\hbar} S_l(\underline{q})\right), \quad (2)$$

with $S_l(\underline{q}) = \int_{\underline{q}_0}^{\underline{q}} \underline{p}_l(\underline{q}') d\underline{q}'$, where $\underline{p}_l(\underline{q})$ is a preimage of \underline{q} under the projection

$$\pi_N : \mathbb{T}^N \rightarrow \mathbb{R}^N$$

and the sum is over all these preimages. This can be applied for instance to a particle of mass $m=1$ moving in a potential $V = V(\underline{q})$ in \mathbb{R}^N with completely integrable

Hamilton function $H(\underline{p}, \underline{q}) = \frac{p^2}{2} + V(\underline{q})$, whose Hamilton operator $\hat{H}_\hbar = -\frac{\hbar^2}{2} \Delta + V(\underline{q})$ defines a self-adjoint linear operator in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^N)$. It turns out that the amplitude $A_l(\underline{q})$ and therefore the function ψ has singularities at the so called caustic points, which are the images of the singular points of the projection π_N (Berry, 1983). For instance in the case $N=1$ and the Hamilton function $H(q, p) = \frac{p^2}{2m} + V(q)$ one finds for the amplitude $A(q) \sim |E - V(q)|^{-\frac{1}{4}}$. To get solutions of the Schrödinger equation without singularities, according to Maslov's theory, which generalizes the so called connecting formulas of the JWKB solution in dimension $N=1$ at the classical turning points $E = V(q)$, one has to construct also analogous functions $\psi_{\underline{p}}$ in momentum space \underline{p} or some mixed N -dimensional $(q_1, \dots, q_i, p_{i+1}, \dots, p_N)$ - space, whose inverse Fourier transforms determine smooth functions at the caustics. Remains only to glue all these functions together at the caustics in the phase space (Lazutkin, 1993). This gluing process and single valuedness lead finally to corrected quantization conditions of the form (Lazutkin, 1993).

$$\oint_{\gamma_i} \underline{p} d\underline{q} = (n_i + \frac{m_i}{4})h, \quad n_i \in \mathbb{N}, \quad 1 \leq i \leq N, \quad (3)$$

where the integers m_i , the Maslov indices of the closed paths γ_i , are determined by the way γ_i passes through the singular set of the projection map $\pi_N : \mathbb{T}^N \rightarrow \mathbb{R}^N$. To get this way solutions of the Schrödinger equation at least up to order \hbar^2 the amplitude functions A_l have to fulfill so called transport equations, which determine them uniquely up to a multiplicative constant (Lazutkin, 1993). Obviously these quantization conditions determine via the paths $\gamma_i, 1 \leq i \leq N$ an invariant torus \mathbb{T}_\hbar^N and hence also an energy value E_\hbar of the classical Hamilton function H with $H|_{\mathbb{T}_\hbar^N} = E_\hbar$. It is known, that these values are indeed approximate eigenvalues of the Schrödinger operator (Lazutkin, 1993), whereas in general only linear combinations of the above quasimodes ψ , constructed via the invariant tori, determine approximate eigenfunctions (Lazutkin, 1993; Jakobson and Zelditch, 1999). According to the KAM Theorem of Kolmogorov, Arnold and Moser invariant tori exist also for weak perturbations of completely integrable systems, which can be used to determine this way at least part of the spectrum of the Schrödinger operator for such systems (Lazutkin, 1993). By construction, the quasimodes "concentrate" in a certain sense to be explained later, around these invariant tori \mathbb{T}_\hbar^N in the energy shell Γ_{E_\hbar} of the classical phase space.

1.4.2. The Weyl Quantization and Wigner's Distribution

In a classically chaotic system, as for instance an ergodic Hamiltonian system, on the other hand a generic orbit covers densely the whole energy shell Γ_E . This led Berry

(1983) to his general semiclassical eigenfunction hypothesis. To formulate this hypothesis, consider the phase space distribution $W_\psi(\underline{q}, \underline{p})$ introduced in 1932 by E. Wigner for any quantum state ψ in the Hilbert space $L^2(\mathbb{R}^N)$ of a system with N degrees of freedom, and defined as

$$W_\psi(\underline{q}, \underline{p}) = \frac{1}{(2\pi\hbar)^N} \int_{\mathbb{R}^N} d\underline{x} \exp\left(-i\frac{\underline{p}\cdot\underline{x}}{\hbar}\right) \psi^*\left(\underline{q} - \frac{\underline{x}}{2}\right) \psi\left(\underline{q} + \frac{\underline{x}}{2}\right). \quad (4)$$

Then, according to Berry's eigenfunction hypothesis, each semiclassical eigenstate ψ_\hbar for $\hbar \rightarrow 0$ should have a Wigner distribution $W_{\psi_\hbar}(\underline{q}, \underline{p})$ which is concentrated on the region of phase space explored over infinite time by a typical orbit of the corresponding classical system, that means, on an invariant torus for a classically completely integrable system, respectively on the entire energy shell for a classically ergodic system. In the latter case, the Wigner distribution of a normalized eigenstate $\psi_\hbar = \psi_\hbar(\underline{q})$ then has the form

$$W_{\psi_\hbar}(\underline{q}, \underline{p}) \approx \frac{\delta(E - H(\underline{q}, \underline{p}))}{\int_{\Gamma} d\underline{q} d\underline{p} \delta(E - H(\underline{q}, \underline{p}))}.$$

Furthermore he suggested, that the individual semiclassical eigenstates ψ_\hbar of classically ergodic systems should behave like Gaussian random fields, that means random functions of several variables, whose finite dimensional distributions

$$F_{\underline{q}_1, \dots, \underline{q}_k}(x_1, \dots, x_k) = \text{Prob}\{\psi(\underline{q}_1) \leq x_1, \dots, \psi(\underline{q}_k) \leq x_k\}$$

are multivariate Gaussian functions for all $\underline{q}_1, \dots, \underline{q}_k$ and arbitrary $k \in \mathbb{N}$ (Berry, 1977). Such Gaussian random fields can be constructed for instance by superposing a large number of plane waves with uniformly distributed random phases. This random wave model has been checked experimentally for certain microwave resonators (Stöckmann, 2006)

Even if semiclassical quantum mechanics has a rigorous foundation in the theory of pseudo-differential operators and Fourier integral operators (Zworski, 2012), there are few rigorous results concerning the above formulated conjectures for general quantum systems with either completely integrable or chaotic classical limit.

1.4.3. Trace Formulas

There do not exist many methods which allow one to relate classical and quantum physics: one of them are trace formulae like Selberg's trace formula (Selberg, 1954) or Gutzwiller's semiclassical trace formula (Gutzwiller, 1991; Combescure et al, 1999), which connect the periodic orbits of a classical chaotic Hamiltonian flow with the trace of its Hamilton operator. To get the flavor of such trace formulas, consider a particle

moving freely on a compact surface M of constant negative curvature, which we will discuss in more detail in Section 3.1. The corresponding chaotic Hamiltonian flow is the geodesic flow on this surface, whereas its Hamilton operator in units, where $-\frac{\hbar^2}{2m} = 1$, is the hyperbolic Laplace-Beltrami operator $\Delta := \Delta_{hyp} = -y^{-2}(\partial_x^2 + \partial_y^2)$. If $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \dots \rightarrow \infty$ denote its eigenvalues and l_γ is the length of a prime periodic orbit γ of the flow, then the Selberg trace formula for this system has the following form (see for instance (Marklof, 2012)):

$$\sum_{j=0}^{\infty} h(\rho_j) = \frac{\text{Area}(M)}{4\pi} \int_{-\infty}^{\infty} h(\rho) \tanh(\pi\rho) \rho d\rho + \sum_{\gamma} \sum_{n=1}^{\infty} \frac{l_{\gamma} g(nl_{\gamma})}{2 \sinh(\frac{nl_{\gamma}}{2})}$$

Thereby $\rho_j = \sqrt{\lambda_j - \frac{1}{4}}$ and h denotes an even function on the complex z plane analytic in the strip $|\text{Im } z| \leq \sigma, \sigma > \frac{1}{2}$, and decaying fast enough at infinity, so that the infinite sum over the eigenvalues converges, respectively g denotes the Fourier transform of h . Obviously, it is not straightforward to extract from such a trace formula the local statistics of the eigenvalues or the morphology of the eigenfunctions. It is therefore not surprising, that most of the rigorous results in the theory of quantum chaos have been obtained by completely different methods, unknown before to the quantum physics community, which however can be applied only for a special class of systems. These are systems, whose classical phase space and dynamics have nice arithmetic properties and their behavior in the semiclassical limit is closely related to known problems in number theory. A typical example is the above mentioned geodesic flow on a surface of constant negative curvature and its quantization, the Laplace-Beltrami operator. Its spectrum is known to be directly related to the theory of automorphic and modular functions for the Fuchsian group defining the surface (Sarnak, 1997) and well studied in analytic and algebraic number theory. Such systems belong to a special branch of quantum chaos, so called arithmetic quantum chaos. Another class of systems also belonging to this branch, are quantized symplectic maps of symplectic manifolds like the so called cat map of the 2-torus, which we will discuss later.

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Biographical Sketch

D. H. Mayer received both his Diploma in Physics and the degree Dr. rer. nat. from the University of Munich, the latter in 1972. He was assistant professor in Theoretical Physics at the Aachen Institute of Technology, and as a research fellow of the German Science Foundation (DFG) a postdoc at the Institute des Hautes Etudes Scientifiques (IHES) at Bures sur Yvette (France) and the Simon Frazer University at Vancouver (Canada). After his Habilitation in Theoretical Physics at the Aachen Institute of Technology in 1979 he became a Heisenberg Fellow of the German Research Foundation with research stays at the IHES and the Mathematics Department of Warwick University. He replaced full professorships in Mathematics at the University of Heidelberg and in Theoretical respectively Mathematical Physics at the Aachen Institute of Technology and at the Universities of Essen and Giessen. After several visiting professorships at the Research Center Juelich, the IHES in Bures sur Yvette and the Max Planck Institute for Mathematics in Bonn he became in 1991 Professor of Theoretical Physics at the University of Clausthal. There he served as Dean of the Physics Department and of the Faculty for Natural Sciences. After his retirement in 2008 he got a Lower Saxony Professorship for Dynamical Systems, Automorphic Spectral Theory and Number Theory at the University of Clausthal. His interests include the thermodynamic formalism in classical statistical mechanics and the theory of dynamical systems, dynamical and number theoretic zeta functions, the transfer operator approach to quantum chaos and automorphic spectral theory respectively the ergodic theory of circle maps with singularities.