Spectral Statistics

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Abstract. The relation between statistical properties of energy eigenvalues of deterministic systems and the distribution of periodic orbits is discussed.

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1 Introduction

The purpose of this paper is to attract attention to the subject of statistical distribution of deterministic sequences. In quantum chaos problems they can be the eigenvalues of a quantum mechanical problem, in number theory the natural choice is the imaginary parts of non-trivial zeros of zeta functions, etc.

The important point that makes this field interesting is the observation that statistical distributions of completely different sequences are, to a large extent, universal depending only on very robust properties of the system considered. The origin of such universal laws remains unclear.

In the fifties Wigner and later Dyson (see articles in [1] and the review [2]), based on a physical idea that 'complicated' means 'random', have proposed to consider the Hamiltonian of heavy nuclei as a random matrix taken from a certain ensemble characterized only by symmetry properties. The duality: 'Hamiltonian $\longleftrightarrow$ random matrix' has been proved very useful [3], [4] and stimulated the development of random matrix theory [5]. Later it was understood that the same idea can also be applied to low-dimensional quantum systems and the accepted conjectures are: (i) local statistical behaviour of energy levels of classically integrable systems is close to the Poisson distribution [7], (ii) energy levels of classically chaotic systems are distributed as eigenvalues of random matrices from the standard random matrix ensembles [6]. One of these ensembles (Gaussian Unitary Ensemble (GUE)) seems to describe the local spectral distribution of non-trivial zeros of zeta functions of number theory [8]-[11].

The volume of numerical evidences in the favor of these conjectures is impressive (see e.g. [3], [9], [4]) but the full mathematical proof even in the simplest cases is still lacking.

In this paper we shall discuss a straightforward method to attack this problem based on trace formulae.

2 Trace formulae

The Gutzwiller trace formula [12] states that the density of eigenvalues for a quantum system can be written as a sum of a smooth ($\bar{d}$) term and an oscillating part

$$d^{(osc)}(E) = \sum_{ppo} \sum_{n=1}^{\infty} A_{p,n} \exp(\frac{i}{\hbar} n S_p(E)) + c.c. \ , \tag{1}$$

given by a sum over primitive periodic orbits and their repetitions. Here S_p is the classical action calculated along one of such orbits,

$$A_{p,n} = \frac{T_p}{2\pi\hbar |Det(M_p^n - 1)|^{1/2}} \exp(-i\frac{\pi}{2} n \mu_p),$$

M_p is the monodromy matrix around the orbit, T_p is its period, and μ_p is the Maslov index. For the motion on constant negative curvature surfaces generated by discrete groups this formula coincides with the Selberg trace formula but for generic systems it represents only the first term of a formal expansion on the Planck constant.

Similar expresion exists also for the Riemann zeta function. For the density of nontrivial Riemann zeros (assuming $s_n = \frac{1}{2} + iE_n$)

$$d^{(osc)}(E) = -\frac{1}{\pi} \sum_{n=1}^{\infty} \frac{1}{\sqrt{n}} \Lambda(n) \cos(E \log n), \tag{2}$$

where $\Lambda(n) = \log p$, if n is a power of a prime p, and $\Lambda(n) = 0$ otherwise.

3 Correlation functions

The n-point correlation function of energy levels is defined as the probability of having n levels at prescribed positions

$$R_n(\epsilon_1, \epsilon_2, \dots, \epsilon_n) = < d(E+\epsilon_1) d(E+\epsilon_2) \dots d(E+\epsilon_n) >, \tag{3}$$

where the brackets $< \dots >$ denote the smoothing over an energy window

$$< f(E) > = \int f(E') \sigma(E - E') dE', \tag{4}$$

with an appropriate weighting function $\sigma(E)$ centered near zero.

In particular, the 2-point correlation function has the form

$$\begin{aligned} R_2(\epsilon_1, \epsilon_2) \qquad &= \bar{d}^2 + \sum_{p_i, n_i} A_{p_1,n_1} A^*_{p_2,n_2} < \exp(\frac{i}{\hbar}(n_1 S_{p_1}(E) - n_2 S_{p_2}(E))) > \\ &\times \exp(\frac{i}{\hbar}(n_1 T_{p_1}(E)\epsilon_1 - n_2 T_{p_2}(E)\epsilon_2)) + c.c. \end{aligned} \tag{5}$$

The terms with the sum of actions are assumed to be washed out by the smoothing procedure.

4 Diagonal approximation

Berry in [13] proposed to estimate the above sum by taking into account only terms with exactly the same actions which leads to the following expression for the two-point correlation form factor (the Fourier transform of R_2)

$$K^{(diag)}(t) = 2\pi \sum_{p,n} |A_{p,n}|^2 \delta(t - nT_p(E)) + c.c., \tag{6}$$

where the sum is taken over all periodic orbits with exactly the same action.

Using the Ruelle-Bowen-Sinai measure on periodic orbits (called in physical literature the Hannay-Ozorio de Almeida sum rule [14]) one finds that for ergodic systems

$$K^{(diag)}(t) = g\frac{t}{2\pi}, \tag{7}$$

where g is the mean multiplicity of periodic orbits. For generic systems without time reversal invariance $g = 1$ and for systems with time reversal invariance $g = 2$ and this result coincides with the small-t behaviour of form factor of classical ensembles.

Unfortunately, $K^{(diag)}(t)$ grows with t but the exact form factor for systems without spectral degeneracies should tend to $\bar{d}$ when $t \to \infty$. This contradiction clearly indicates that the diagonal approximation cannot be correct for all values of t and more complicated tools are needed to obtain the full form factor.

5 Beyond the diagonal approximation

We begin to discuss the calculation of off-diagonal terms on the example of the Riemann zeta function where more information is available and then we shall generalize the method to dynamical systems.

The connected two-point correlation function of the Riemann zeros is

$$R_2(\epsilon_1, \epsilon_2) = \frac{1}{4\pi^2} \sum_{n_1,n_2} \frac{\Lambda(n_1)\Lambda(n_2)}{\sqrt{n_1 n_2}} < e^{iE\log(n_1/n_2) + i(\epsilon_1 \log n_1 - \epsilon_2 \log n_2)} > +c.c. \tag{8}$$

The diagonal terms correspond to $n_1 = n_2$ and

$$R_2^{(diag)}(\epsilon) = -\frac{1}{4\pi^2}\frac{\partial^2}{\partial\epsilon^2} \log(|\zeta(1+i\epsilon)|^2 \Phi^{(diag)}(\epsilon)), \tag{9}$$

where $\epsilon = \epsilon_1 - \epsilon_2$ and the function $\Phi^{(diag)}(\epsilon)$ is given by a convergent sum over prime numbers

$$\Phi^{(diag)}(\epsilon) = \exp(-\sum_p \sum_{m=1}^{\infty} \frac{m-1}{m^2 p^m} e^{im\log p\epsilon} + c.c.). \tag{10}$$

When $\epsilon \to 0$, $R_2(\epsilon) \to -(2\pi^2\epsilon^2)^{-1}$ which agrees with the smooth GUE result.

The term $\exp(iE\log(n_1/n_2))$ oscillates quickly if n_1 is not close to n_2. Denoting $n_1 = n_2 + h$ and expanding smooth functions on h one gets

$$R_2^{(off)}(\epsilon) = \frac{1}{4\pi^2} \sum_{n,d} \frac{\Lambda(n)\Lambda(n+h)}{n} < e^{iE(h/n)+i\epsilon\log n} > +c.c. \tag{11}$$

The main problem is clearly seen here. The function $F(n,h) = \Lambda(n)\Lambda(n+h)$ changes irregularly as it is nonzero only when both n and $n+h$ are powers of prime numbers. Fortunately, the dominant contribution to the two-point correlation function comes from the mean value of this function

$$\alpha(h) = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \Lambda(n)\Lambda(n+h), \tag{12}$$

and its explicit expression follows from the famous Hardy–Littlewood conjecture [15]

$$\alpha(h) = \sum_{(p,q)=1} e^{-2\pi i \frac{p}{q} h} \left(\frac{\mu(q)}{\psi(q)} \right)^2, \tag{13}$$

where the sum is taken over all coprime integers q and $p < q$, $\mu(n)$ and $\psi(n)$ are the Mobius and the Euler functions respectively.

Using this expression for $\alpha(h)$ and performing the sum over all h one obtains

$$R_2^{(off)}(\epsilon) = \frac{1}{4\pi^2} |\zeta(1+i\epsilon)|^2 e^{2\pi i \bar{d}\epsilon} \Phi^{(off)}(\epsilon) + c.c., \tag{14}$$

where function $\Phi^{(off)}(\epsilon)$ is given by a convergent product over primes

$$\Phi^{(off)}(\epsilon) = \prod_p (1 - \frac{(1-p^{i\epsilon})^2}{(p-1)^2}). \tag{15}$$

In the limit of small ϵ, $R_2^{(off)}(\epsilon) \to (e^{2\pi i\bar{d}\epsilon} + e^{-2\pi i \bar{d}\epsilon})/(2\pi\epsilon)^2$ which corresponds exactly to the GUE result.

The above calculations demonstrate how one can compute the two-point correlation function through the knowledge of pair-correlation function of periodic orbits. For the Riemann case one can prove under the same conjectures[1] that all n-point correlation functions of Riemann zeros tend to the corresponding GUE results [16].

The interesting consequence of the above formula is the expression for the two-point form factor

$$K^{(off)}(t) = \frac{1}{4\pi^2} \sum_{(p,q)=1} \left(\frac{\mu(q)}{\psi(q)} \right)^2 (\frac{q}{p}) \delta(t - 2\pi\bar{d} - \log\frac{q}{p}), \tag{16}$$

which means that the off-diagonal two-point form factor is a sum over δ-functions in special points equal the Heisenberg time ($T_H = 2\pi\bar{d}$) plus a difference of periods

[1] Really only a smoothed version of the Hardy-Littlewood conjecture is needed.

of two pseudo-orbits (linear combinations of periodic orbits). This set is dense but the largest peaks correspond to the shortest pseudo-orbits. Similarly the two-point diagonal form factor is the sum of δ functions at the positions of periodic orbits

$$K^{(diag)}(t) = \frac{1}{4\pi^2} \sum_{p,m} \frac{\log^2 p}{p^m} \delta(t - m \log p). \tag{17}$$

The smooth values corresponding to the random matrix predictions appear only after a smoothing of these functions over a suitable interval of t.

6 Arithmetical systems

Similar behavior has been observed in a completely different model, namely for the distribution of eigenvalues of the Laplace–Beltrami operator for the modular domain [17]. It was shown that in this model the two-point correlation form factor can be written in the following form

$$K(t) = \frac{1}{\pi^3 k} \sum_{(p,q)=1} \left| \frac{q}{p} \beta(p,q) \right|^2 \delta(t - t_{p,q}), \tag{18}$$

where

$$t_{p,q} = \frac{2}{k} \ln \frac{kq}{\pi p}, \text{ and } \beta(p,q) = \frac{S(p,p;q)}{q^2 \prod_{\omega|q}(1 - \omega^{-2})}.$$

The product is taken over all prime divisors of q and $S(p,p;q)$ is the Kloosterman sum

$$S(n,m;c) = \sum_{d=1}^{c-1} \exp(2\pi i (nd + md^{-1})/c).$$

This model belongs to the so-called arithmetical models corresponding to the motion on constant negative curvature surfaces generated by arithmetic groups. For all these models due to the exponential multiplicities of periodic orbits one expects [18] that the spectral statistics will tend to the Poisson distribution though from a classical point of view all these models are the best known examples of classically chaotic motion. Using the above expression one can prove this statement for the modular group.

7 Construction of the density of states from finite number of periodic orbits

The main difficulty in using trace formulae is their divergent character. The diagonal approximation consists, in some sense, on computing the density of states from a sum over a finite number of periodic orbits but this sum cannot produce δ-function singularities. There exists an artificial method [19] which permits to avoid this difficulty. Its main ingredient is the Riemann-Siegel form of the zeta function

$$\zeta(1/2 - iE) = z_T(E) + e^{2\pi i \bar{N}(E)} z_T^*(E), \tag{19}$$

where instead of the correct Riemann-Siegel expansion one uses a truncated product over periodic orbits

$$z_T(E) = \prod_{\log p < T} (1 - p^{-1/2+iE})^{-1}.$$

The density of zeros for function (19) takes the form

$$D_T(E) = d_T(E) \sum_{k=-\infty}^{\infty} (-1)^k e^{2\pi i k \bar{N}(E)} \left(\frac{z_T^*(E)}{z_T(E)} \right)^k , \tag{20}$$

where $d_T(E)$ is the density of state truncated at $\log p < T$.

Assuming that T is of the order of the Heisenberg time, $T_H = 2\pi \bar{d}$, and $\bar{d} \to \infty$ after some algebra we get

$$R_2^{(off)}(\epsilon_1, \epsilon_2) = \bar{d}^2 e^{2\pi i \bar{d}\epsilon} < \frac{z_T^*(E+\epsilon_1) z_T(E+\epsilon_2)}{z_T(E+\epsilon_1) z_T^*(E+\epsilon_2)} > + c.c. \tag{21}$$

The last step consists in performing the energy average of this expression. As logarithms of primes are not commensurable, the energy average of any smooth function of $\exp(iE \log p_j)$ equals its phase average

$$< f >= \int_0^{2\pi} \dots \int_0^{2\pi} f(e^{i\phi_1}, \dots, e^{i\phi_M}) \prod_{j=1}^{M} \frac{d\phi_j}{2\pi}. \tag{22}$$

This is essentially equivalent to the random phase approximation, or to the ergodic theorem for quasi-periodic functions with non-commensurable periods, or to the strict diagonal approximation.

For the Riemann zeta function the total contribution equals

$$R_2(\epsilon) = C^2 \exp(2\pi i \bar{d}\epsilon) |\zeta(1+i\epsilon)|^2 \Phi^{(off)}(\epsilon) + c.c. \,, \tag{23}$$

where

$$\Phi^{(off)}(\epsilon) = \prod_p (1 - \frac{(1-p^{i\epsilon})^2}{(p-1)^2}), \tag{24}$$

$\epsilon = \epsilon_2 - \epsilon_1$, and $C = \bar{d} \prod_p (1 - 1/p)$. All products in these expressions include prime numbers up to $\ln p = T$. The first two products converge when $T \to \infty$ and only the last one requires a regularization. But our parameter T has not yet been fixed. Let us choose it in such a way that

$$2\pi \bar{d} \prod_{\ln p < T} (1 - \frac{1}{p}) = 1. \tag{25}$$

The same factor appears in the statistical approach to prime numbers (see discussion in [15]) and can be considered as a renormalisation of formally divergent sums. After this renormalization we get exactly the same formula (14) as has been derived in the previous section using the Hardy-Littlewood conjecture about the pairwise distribution of prime numbers.

8 Off-diagonal terms for dynamical systems

For 2-dimensional dynamical systems the only difference with the Riemann case is that the truncated zeta function $z_T(E)$ contains now an infinite product over m

$$z_T(E) = \prod_{T_p<T} \prod_{m=0}^{\infty} (1 - \frac{e^{iS_p(E)/\hbar - i\pi\mu_p/2}}{|\Lambda_p|^{1/2}\Lambda_p^m}), \tag{26}$$

where Λ_p is the largest eigenvalue of the monodromy matrix.

The simplest and most natural assumption is that in generic systems without time-reversal invariance periodic orbits up to period T are linearly non-commensurable (as primes). Under this conjecture after some algebra we obtain that when $T \to \infty$

$$R_2(\epsilon) = \frac{e^{2\pi i \bar{d}\epsilon}}{4\pi^2} |\gamma^{-1} Z_{cl}(i\epsilon)|^2 \prod_p < R_p > \left| \frac{Z_p(i\epsilon)}{Z_p(0)} \right|^2 + c.c. \tag{27}$$

and

$$< R_p >= \sum_{n=0}^{\infty} \frac{(a;q)_n^2}{(q;q)_n^2} y^n, \tag{28}$$

where $(a;q) = (1-a)(1-aq)\ldots(1-aq^{n-1})$, $a = e^{-i\tau_p}$, $q = \Lambda_p^{-1}$, $y = |\Lambda_p|^{-1} e^{i\tau_p}$, and $\tau_p = l_p \epsilon / k$. $Z_{cl}(s)$ is a classical zeta function, $Z_{cl}(s) = \prod_p Z_p(s)^{-1}$ with $Z_p(s) = 1 - e^{\tau_p s}/|\Lambda_p|$.

The maximum period T is determined from the condition

$$2\pi \bar{d} \prod_{T_p<T} Z_p(0) = \frac{1}{|\gamma|}, \tag{29}$$

where γ is the residue of $Z_{cl}(s)$ at $s = 0$ ($Z_{cl}(s) \to \gamma/s$ when $s \to 0$). As above this renormalization fixes T to be of the order of T_H and ensures that, when $\epsilon \to 0$, $R_2(\epsilon)$ tends to the GUE result.

9 Random matrix universality

There exists another method of semiclassical calculation of off-diagonal part of correlation functions which demonstrates that if such formulae exist they coincide with the above obtained expressions.

According to the naive trace formula the density of states is

$$d(E) = \tilde{d}(E) + \eta(E), \tag{30}$$

where $\tilde{d}(E)$ is the truncated density of states computed from a set of short-period orbits with period $T_p < T$ (now we shall assume that $T \ll T_H$) and $\eta(E)$ is (unknown) part of the density constructed from high-period orbits.

Let us try now to construct a random matrix ensemble which has the mean density of eigenvalues exactly equals $\tilde{d}(E)$. In principle, the necessary potential can be computed from the Dyson equation

$$\int \frac{\tilde{d}(t)}{x-t} dt = \frac{1}{2} V'(x). \tag{31}$$

But the explicit form of this potential is irrelevant as under quite general conditions the resulting distribution does not depend on the explicit form of this function (provided it corresponds to the so-called definite momentum problem [21]) and all correlation functions depend only on the kernel $K_N(x,y)$ which in the bulk of the spectrum in the limit $N \to \infty$ tends to

$$K(x,y) = \frac{\sin \pi (N(x) - N(y))}{\pi(x-y)}, \tag{32}$$

where $N(x) = \int^x \tilde{d}(x')dx'$ is the mean staircase function.

Hence, the two-point correlation function will take the form

$$R_2(\epsilon_1, \epsilon_2) = < \tilde{d}(E+\epsilon_1)\tilde{d}(E+\epsilon_2) - \frac{\sin^2 \pi(\tilde{N}(E+\epsilon_1) - \tilde{N}(E+\epsilon_2))}{\pi^2(\epsilon_1 - \epsilon_2)^2} > . \tag{33}$$

As $\tilde{d}(E)$ is known it is possible to perform the smoothing over the appropriate energy window. Using the same transformations as above one can show that under the assumption $T \ll T_H$ the dependence of T will disappear and one gets the same formulae as above.

10 Conclusion

The heuristic arguments presented in this paper demonstrate how, in principle, the existence of the trace formula and certain natural conjectures about the distribution of periodic orbits (or primes) combine together to produce universal local statistics. In particular, for systems without the time-reversal invariance the assumption that low-period orbits are non-commensurable leads to the GUE statistics (at least for 2-point correlation function). The close relation between diagonal (9) and off-diagonal (14) terms (first observed for disordered systems in [22]) suggests the existence of a certain unified principle. The best candidate for it is the 'unitarity' property of the trace formula, namely, that the distribution of periodic orbits should be such that the corresponding eigenvalues will be real. In some sense certain long-period orbits are connected to the short ones and the investigation of this connection may clarify the origin of universal spectral statistics. The interesting question is what conjectures about periodic orbits are necessary to obtain correlation functions for systems with time-reversal invariance where almost all periodic orbits appear in pairs with exactly the same action.

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