Level spacings and periodic orbits

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Starting from a semiclassical quantization condition based on the trace formula, we derive a periodic-orbit formula for the distribution of spacings of eigenvalues with k intermediate levels. Numerical tests verify the validity of this representation for the nearest-neighbor level spacing ($k=0$). In a second part, we present an asymptotic evaluation for large spacings, where consistency with random matrix theory is achieved for large k. We also discuss the relation with the method of Bogomolny and Keating [Phys. Rev. Lett. **77**, 1472 (1996)] for two-point correlations.

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The statistical distribution of quantum energy levels is conjectured to reflect the chaoticity or integrability of the underlying classical dynamics [1,2]. For classically chaotic systems one expects spectral distributions like those computed in random matrix theory (RMT) [2], whereas for classically integrable systems the quantum levels appear to follow the distribution for a Poisson process [1]. Attempts to explain this correspondence are based on Gutzwiller's semiclassical trace formula [3] which bridges the gap between classical and quantum mechanics. The prime result in this direction is Berry's analysis of the spectral rigidity [4], based on the so-called diagonal approximation and the classical sum rule of Hannay and Ozorio de Almeida [5]. Starting from a semiclassical quantization condition [6,7], Bogomolny and Keating [8] were able to extract information on the two-point correlations going beyond the results of Ref. [4]. It is the aim of the present paper to follow a similar path in order to obtain semiclassical information on the level spacing distributions.

The Gutzwiller trace formula can be expressed as a periodic-orbit sum for the integrated density of states $N(E) := \sum_n \Theta(E-E_n)$,

$$N_T(E) \sim \overline{N}(E) + \mathrm{Re} \sum_{T_\gamma \leqslant T} \mathcal{A}_\gamma e^{(i/\hbar) S_\gamma(E)}, \tag{1}$$

in the semiclassical limit, i.e., for $\hbar \to 0$. $\overline{N}(E)$ denotes the mean part following from Weyl's law, whereas the fluctuations $N_T^{\mathrm{fl}}(E)$ are given by a sum over all periodic orbits γ of the corresponding classical system. The action and period of a periodic orbit are denoted by $S_\gamma(E)$ and $T_\gamma(E)$, respectively. The explicit form of the amplitudes $\mathcal{A}_\gamma$ can be found in [3] for chaotic and in [9] for integrable systems. We have given a version truncated at periods $T_\gamma = T$, which will be needed in the following. Instead of directly using Eq. (1) to express spectral functions, we will use an approximate spectrum $E_n(T)$ obtained from the condition [6,7]

$$N_T(E_n(T)) \overset{!}{=} n + \tfrac{1}{2}. \tag{2}$$

Before investigating the statistical distribution we have to unfold the spectrum such that its mean density $\overline{d}(E) = d\overline{N}(E)/dE$ is rescaled to unity. To this end, investigating spectral correlations in an interval $I(E;\hbar) := [E-\hbar\omega, E+\hbar\omega]$, we introduce the unfolded energies $x_n(T) := E_n(T)\overline{d}$, $\overline{d} := \overline{d}(E)$, see, e.g., [10] for details. Spacings of two unfolded energies with k intermediate levels are given by $s_n(k;T) = x_{n+k+1}(T) - x_n(T)$ and integrated level spacing distributions are defined by

$$I(k,s;T) := \frac{1}{N_I} \sum_{E_n \in I(E;\hbar)} \Theta(s - s_n(k;T)), \tag{3}$$

where N_I denotes the number of eigenvalues contained in $I(E;\hbar)$. The often used level spacing densities $P(k,s;T)$ are the derivative of $I(k,s;T)$ with respect to s. Since the condition $s \geqslant s_n(k;T)$ can be rewritten as $N_T(E_n(T)+s/\overline{d}) - N_T(E_n(T)) \geqslant k$, we can substitute the argument of the step function. Upon replacing the sum by an integral over $I(E;\hbar)$ with weight $d(E')$ which, in turn, we can asymptotically substitute by $d_T(E') := dN_T(E')/dE'$ we obtain

$$I(k,s;T) \sim \left\langle \Theta\left[N_T\left(E' + \frac{s}{\overline{d}}\right) - N_T(E') - k - 1 \right] \frac{d_T(E')}{\overline{d}} \right\rangle. \tag{4}$$

The brackets denote the energy average $\langle \dots \rangle := (2\hbar\omega)^{-1} \int_{E-\hbar\omega}^{E+\hbar\omega} \dots dE'$, due to which we may asymptotically replace $d_T(E')/\overline{d}$ by 1. Since the semiclassical limit $\hbar \to 0$ now implies $\overline{d} \to \infty$, we have $s/\overline{d} \ll 1$, and expanding the mean part of N_T about E yields the periodic-orbit formula

$$I(k,s;T) \sim \left\langle \Theta\left(s - k - 1 + N_T^{\mathrm{fl}}\left(E' + \frac{s}{\overline{d}}\right) - N_T^{\mathrm{fl}}(E') \right) \right\rangle \tag{5}$$

for the integrated level spacing distribution. A similar expression can be obtained for the level spacing distribution $P(k,s;T)$ itself by taking the derivative of Eq. (5). Here we again neglect $d_T^{\mathrm{fl}}(E' + s/\overline{d})/\overline{d}$ because of the energy average, i.e.,

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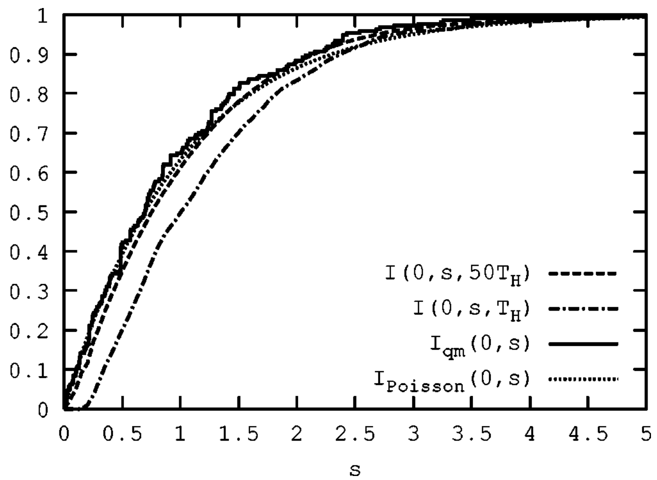

FIG. 1. Integrated level spacing distribution from periodic orbits Eq. (5) for a rectangular billiard with cutoff time $50T_H$ (dashed) and T_H (dashed-dotted). The quantum mechanical level spacing distribution (solid) and the graph for a Poisson process (dotted) are shown for comparison.

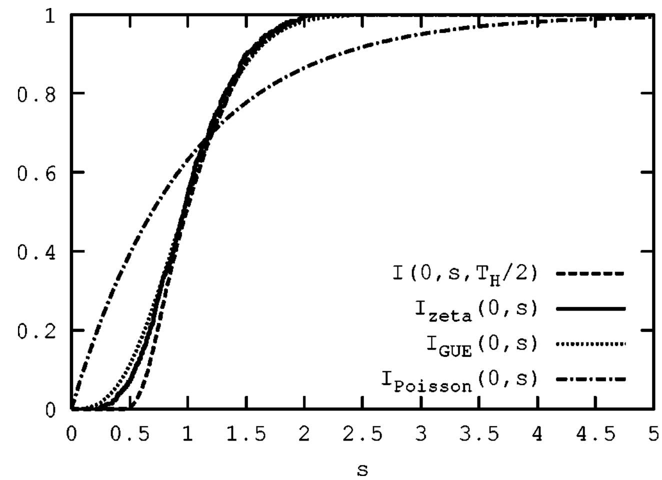

FIG. 2. Integrated level spacing distribution for the zeros of the Riemann zeta function (solid) and the spacing distribution calculated from prime numbers (dashed), cf. Eq. (5), $T=T_H/2$. The spacing distribution of the GUE (dotted) and for a Poisson process (dashed-dotted) are shown for comparison.

$$P(k,s;T)\sim\left\langle \delta\left[s-k-1+N_T^{\mathrm{fl}}\left(E'+\frac{s}{\bar{d}}\right) -N_T^{\mathrm{fl}}(E')\right]\right\rangle . \tag{6}$$

For the most intensively studied case $k=0$, i.e., for nearest-neighbor level spacings, we will now test these formulas numerically for two toy models. Our first example is a classically integrable system, namely a rectangular quantum billiard with aspect ratio $2/(1+\sqrt{5})$ and Neumann boundary conditions. For scaling systems the semiclassical limit $\hbar\to 0$ can be replaced by the high energy limit $E\to\infty$, with a suitable change in the energy average. For the plots we have taken into account energies in the interval $E\in[0,4000]$ (corresponding to 214 eigenvalues). Figure 1 shows the integrated level spacing distribution for this system where for the cutoff time T we have chosen $T=T_H:=2\pi\hbar\bar{d}$ (dashed-dotted line) and $T=50\,T_H$ (dashed line), respectively. When increasing the cutoff time T we observe convergence toward the quantum mechanical result (solid line), which in turn in the limit $E\to\infty$ converges to a Poissonian level spacing distribution (dotted line), cf. [11].

For a second test we have chosen the imaginary parts of the nontrivial zeros of the Riemann zeta function. These serve as a model for quantum chaos, since their spectral correlations are well described by the Gaussian unitary ensemble (GUE), see, e.g., [12] and references therein. The density of the Riemann zeros is related to a sum over primes, see, e.g., [13], in a similar way as the density of states of a quantum system is related to a sum over periodic orbits of the corresponding classical system Eq. (1).

In Fig. 2 the integrated level spacing distribution of the first 649 Riemann zeros with imaginary parts between 0 and 1000 (solid line) is shown as well as the analogue of Eq. (5) (dashed line) with a truncation of the sum over primes at the Riemann–Siegel cutoff [14] which corresponds to $T_H/2$ [15]. We observe a good agreement of both curves for large s where both approach the GUE result (dotted line). However, for values of s below 1 the periodic-orbit formula differs from both the GUE and the exact curve. This is due to the fact that the periodic orbit sum Eq. (1), truncated at the order of the Heisenberg time, cannot reproduce features below the scale of mean level spacing. Unlike in the integrable case, by using a sharp cutoff we cannot simply increase T since now the sum over primes numerically behaves like an asymptotically divergent series, i.e., including, e.g., orbits up to the Heisenberg time yields worse results. One could possibly overcome this drawback by using a smoothed and thus convergent trace formula, see [16]. We will not further pursue this approach since it requires a much larger number of orbits (in Fig. 2 only primes up to 13 are needed), which for typical systems are not available. Instead for later reference we only remark that any cutoff, either sharp as above or the effective cutoff in a smoothed trace formula, has to be a multiple of the Heisenberg time.

Now that we have checked the periodic orbit formula numerically, we turn to an asymptotic evaluation of $P(k,s;T)$ for generic quantum systems with chaotic classical limit. A well established conjecture on global eigenvalue statistics [17] states that (after suitable normalization) in the semiclassical limit the value distribution of N_T^{fl} is given by a Gaussian with zero mean. In analogy to [8] we also assume Gaussian behavior for the difference $N_T^{\mathrm{fl}}(E'+s/\bar{d})-N_T^{\mathrm{fl}}(E')$. Although this assumption leads to the correct result in the case of two-point correlations [8,18], we remark that it corresponds to neglecting cross correlations between N_T^{fl} at different arguments which, especially for small s, will become important. Thus, in the limit $s\to\infty$, $s/\bar{d}\to 0$, the energy average in Eq. (6) can be performed approximately, yielding

$$P(k,s;T)\approx\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{(s-k-1)^2}{2\sigma^2}\right) , \tag{7}$$

where the (s-dependent) variance $\sigma^2 := \langle (N_T^{\mathrm{fl}}(E' + s/\bar{d}) - N_T^{\mathrm{fl}}(E'))^2 \rangle$ of the Gaussian is still to be determined. This last step can be done by substituting the trace formula Eq. (1) for N_T^{fl} and employing an expansion in $s/\bar{d}$ (see [18])

$$\sigma^2 \sim \left\langle \left(\mathrm{Re} \sum_{T_\gamma \leq T} \mathcal{A}_\gamma e^{(i/\hbar) S_\gamma} (e^{(i/\hbar) T_\gamma (s/\bar{d})} - 1) \right)^2 \right\rangle. \quad (8)$$

Since $s/\bar{d} \to 0$ the only rapidly oscillating terms in the double sum involve only the actions S_γ. Thus, following the general idea of the diagonal approximation [5,4], in the limit we only keep terms with identical actions, resulting in

$$\sigma^2 \approx g \sum_{T_\gamma \leq T} |\mathcal{A}_\gamma|^2 \left[1 - \cos\left(\frac{s T_\gamma}{\hbar \bar{d}} \right) \right], \quad (9)$$

where g denotes the generic multiplicity of orbits sharing the same action, see [4,10]. Using the classical sum rule [5] we obtain

$$\sigma^2 \approx \frac{g}{\pi^2} \int_0^T \frac{1 - \cos(sT'/\hbar\bar{d})}{T'} dT' \sim \frac{g}{\pi^2} \left[\log\left(\frac{sT}{\hbar \bar{d}} \right) + \gamma \right], \quad (10)$$

γ denoting Euler's constant. We remark that the subleading term of this expansion is not unique at this point, since it is influenced by corrections to the sum rule (which unfortunately are unknown) as well as by the choice of the cutoff time. Therefore, when now setting $T = CT_H = C2\pi\hbar\bar{d}$ we obtain

$$\sigma^2 \approx \frac{g}{\pi^2} (\log s + \alpha). \quad (11)$$

Here α is kept as a free parameter which, however, will not influence the large-s asymptotics. Upon substituting Eq. (11) into Eq. (7) we obtain a semiclassical formula for the level spacing distributions as $s \to \infty$

$$P_{\mathrm{sc}}(k,s) \approx \sqrt{\frac{\pi/(2g)}{\log s + \alpha}} \exp\left(-\frac{\pi^2 (s-k-1)^2}{2g(\log s + \alpha)} \right). \quad (12)$$

Since Eq. (12) is mainly supported around $s \approx k+1$ we may for a moment substitute $\log s$ by $\log(k+1)$ for large k. The formula obtained that way is consistent with a conjecture for $P(k,s)$ from RMT [19], see also [20], which can be adopted to generic quantum systems with chaotic classical limit [21]. However for small k and in particular for nearest-neighbor level spacings Eq. (12) fails to reproduce the RMT results. This has to be understood in the following sense: The asymptotic techniques used are essentially restricted to two-point correlations. Since the mean distance between x_{n+k+1} and x_n is given by $k+1$, the $P(k,s)$ can only be dominated by two-point correlations on scales where $s \approx k+1$. More precisely, in Eq. (6) one can easily see that assuming a Gaussian distribution with zero mean for $N_T^{\mathrm{fl}}(E' + s/\bar{d}) - N_T^{\mathrm{fl}}(E')$ links s and k. Thus an asymptotic evaluation as $s \to \infty$ also implies large k.

We will now investigate the relation of our result Eq. (12) with the method of Bogomolny and Keating for the two-point correlation function $R_2(s)$, which can be represented as the sum

$$R_2(s) := \sum_{k=0}^{\infty} P(k,s) - 1. \quad (13)$$

Substituting Eq. (12) for the level spacing distributions and applying the Poisson summation formula yields

$$R_{2,\mathrm{sc}}(s) \approx \sum_{\nu \in \mathbb{Z} \setminus \{0\}} \frac{1}{2} \exp(-2\pi^2 \nu^2 \sigma^2) \exp(2\pi i \nu s) \times \left[1 + \mathrm{erf}\left(\frac{s - 1 + 2\pi i \nu \sigma^2}{\sqrt{2}\sigma} \right) \right], \quad (14)$$

where σ^2 is given by Eq. (11). The leading terms as $s \to \infty$ derive from $\nu = \pm 1$ (as can be easily seen from the first exponential), i.e.,

$$R_{2,\mathrm{sc}}(s) \approx 2 e^{-2g\alpha} \frac{\cos(2\pi s)}{s^{2g}}. \quad (15)$$

Comparing with the large-s asymptotics of two-point correlation functions of RMT we observe that we have obtained the leading oscillatory contribution, which can be expected from the method of Bogomolny and Keating [8,18], but are missing the term which corresponds to the diagonal approximation of the spectral form factor (see [4,8,22]). The reason for this is that between Eqs. (4) and (6) we have neglected the term $d_T^{\mathrm{fl}}(E') d_T^{\mathrm{fl}}(E' + s/\bar{d})/\bar{d}^2$, which there was consistent, since it can be determined that doing so neither affects the numerics nor changes the large-s asymptotics of Eq. (12). However, in the sum Eq. (13) the diagonal approximation of this term yields the missing term of $R_2(s)$.

In this sense our result for the level spacing distributions (for large k) is in leading order consistent with RMT two-point correlations. Thus, we can now compare Eq. (15) to the respective results from RMT, in order to fix α. For systems without time-reversal symmetry ($g=1$) we have to compare them with the GUE result, see, e.g., [23], thus obtaining $\alpha = \log(2\pi)$. Analogously for time reversal invariant systems ($g=2$) we obtain $\alpha = \log(\sqrt{2}\pi)$ by comparing with two-point correlations of the Gaussian orthogonal ensemble. Thus, with the substitution $\log s \approx \log(k+1)$ for large k we have obtained Gaussians for the $P(k,s)$ with approximate variances

$$\sigma^2(k) \approx \frac{g}{\pi^2} (\log(k+1) + \alpha),$$

which is consistent with expectations from RMT [19,20] and numerical observations for classically chaotic systems [21].

We briefly remark that the reasoning easily carries over to the third universality class, the Gaussian symplectic ensemble. To this end we have to consider trace formulas for particles with half integer spin [24,25]. For time reversal invariant systems one has to take into account Kramers' degeneracy as in [18]. Again using the Gaussian ansatz Eq. (7) and methods of [10] for the calculation of σ^2 we obtain

$$P_{\mathrm{spin}}(k,s) \approx \sqrt{\frac{\pi}{\log s+\alpha}} \exp\left(-\frac{\pi^2(s-k-1)^2}{\log s+\alpha}\right), \quad (16)$$

where the same procedure as above yields $\alpha=\log 8$.

Summarizing, we have derived periodic orbit formulas for the level spacing distributions $P(k,s)$ and $I(k,s)$. Numerical tests show that using purely classical input even the nearest-neighbor spacing distribution can be obtained for both classically integrable and chaotic systems, where in the latter case with present techniques we cannot go below the scale of mean level spacing. In a second part we have presented an asymptotic evaluation of the formulas for large spacings, which yields good approximations, if we restrict ourselves to the case of large k.

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