Degeneracy Moments for the Square Billiard

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We calculate the semiclassical asymptotics of the moments of a function that characterizes the accidental energy level degeneracies of the square billiard. The results quantify the deviations from generic (Poisson) statistics in this spectrum.

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1 Introduction

It has been conjectured that generically, in the semiclassical limit, quantum spectral statistics on the scale of the mean level separation are Poissonian in classically integrable systems [2]. However, integrable systems which do not exhibit Poissonian statistics are also known. One obvious class of examples are simple harmonic oscillators. Others include two-dimensional rectangular billiards in which the square of the aspect ratio is rational.

Recent results [15] imply that these exceptional cases are far more numerous than previously anticipated. This then promotes the question of how the spectral fluctuations can best be characterized in such systems. For harmonic oscillators, this has been investigated using a number of different approaches [2, 13, 3, 4, 14, 6, 11]. Our purpose here is to focus on one (the simplest) rational rectangular billiard, namely the square.

The energy levels in the square billiard, when suitably scaled, are given by

$$E_{m,n} = m^2 + n^2 \,, \tag{1}$$

where the integers m and n satisfy $m \geq 0$ and $n > 0$. The density of states may thus be written

$$d(E) = \sum_{n=1}^{\infty} r_2(n)\,\delta(E-n)\,, \tag{2}$$

the degeneracy function $r_2(n)$ being the number of ways that n can be expressed as a sum of two squares. The fact that in this case the spectral statistics are non-Poissonian is due to a semiclassically increasing density of accidental degeneracies, which cause the level spacings distribution to tend to a delta-function at zero spacing when $E \to \infty$ (see, for example, [5]).

One way to characterize eigenvalue statistics for the square is in terms of the spectral two-point correlation function. This is obviously determined by the two-point correlations of $r_2(n)$. These were calculated explicitly in [5], and shown to exhibit number-theoretical fluctuations about a Poissonian background.

Another way is in terms of the moments of $r_2(n)$. Moments higher than the second are related to higher-than-two-point spectral correlations, and so contain information beyond that previously calculated. Our main result here is a general formula for the leading-order semiclassical ($n \to \infty$) asymptotics of any given moment of $r_2(n)$. The higher moments turn out to be strongly determined by the accidental degeneracies, and hence represent increasingly sensitive measures of the deviations from generic Poissonian form of the spectral statistics.

This paper is structured as follows. In section 2 we outline the general method of calculation. In section 3 we calculate the second, third and fourth moments explicitly. For the second and third moments, we obtain terms in the semiclassical asymptotics beyond the leading order, and compare the results with numerical computations. Finally, in section 4 we derive a general expression for the leading-order asymptotics of any given moment.

2 General method

Our calculation of the moments of $r_2(n)$ will be based on a well-known relationship (see, for example, [9]) between a sum

$$\sigma(X) = \sum_{n \leq X} \xi(n) \tag{3}$$

and its associated Dirichlet series

$$\Xi(s) = \sum_{n=1}^{\infty} \frac{\xi(n)}{n^s} \,. \tag{4}$$

This is that if

$$I(X) = \frac{\sigma(X+\epsilon) + \sigma(X-\epsilon)}{2} \tag{5}$$

is the average of the right- and left-hand limits of the step-discontinuous function $\sigma(X)$, then

$$I(X) = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} \Xi(s) \frac{X^s}{s} \, \mathrm{d}s \,, \tag{6}$$

where the real constant a is large enough to ensure the absolute convergence of the Dirichlet series. The derivation of this equation follows immediately upon interchange of the integral in (6) with the sum in (4).

We define the moments of $r_2(n)$ by

$$M_k(N) = \frac{1}{N}\sum_{n=1}^{N} r_2^k(n)\,. \tag{7}$$

The semiclassical ($N \to \infty$) asymptotics is obtained by forming a Dirichlet series as in (4), then computing the contribution to the integral (6) from the dominant (right-most) pole of the resulting integrand in the complex s-plane. What allows us to do this is the fact that the Dirichlet series can be re-expressed as an Euler-product over the primes. The right-most pole can then be identified, and the residue calculated explicitly.

The Euler product is derived using the following formula for $r_2(n)$. Let q denote the primes, p the primes congruent to 1 modulo 4, and r the primes congruent to 3 modulo 4. The prime decomposition of an integer n may therefore be written uniquely as

$$n = \prod_q q^{m_q(n)} = 2^{m_2(n)} \prod_p p^{m_p(n)} \prod_r r^{m_r(n)}\,. \tag{8}$$

Then [8]

$$r_2(n) = \begin{cases} \prod_p \Big(m_p(n)+1\Big) & \text{if } 2 \mid m_r(n)\ \forall r \\ 0 & \text{otherwise}\,. \end{cases} \tag{9}$$

To give an example, the first moment (i.e. the average of $r_2(n)$) can be calculated using

$$\Xi_1(s) = \sum_{n=1}^{\infty} \frac{r_2(n)}{n^s} \tag{10}$$

$$= \frac{1}{1-\frac{1}{2^s}} \prod_r \frac{1}{1-\frac{1}{r^{2s}}} \prod_p \left[1 + \frac{2}{p^s} + \frac{3}{p^{2s}} + \ldots + \frac{(k+1)}{p^{ks}} + \ldots\right], \tag{11}$$

where the second equality can be checked by first re-expanding the prime products, then using (9). Evaluating the sum in the p-product gives

$$\Xi_1(s) = \frac{1}{1-\frac{1}{2^s}} \prod_r \frac{1}{1-\frac{1}{r^{2s}}} \prod_p \frac{1}{\left(1-\frac{1}{p^s}\right)^2}, \tag{12}$$

and so we recognize that

$$\Xi_1(s) = \zeta(s)L(s)\,, \tag{13}$$

where

$$\zeta(s) = \prod_p \frac{1}{1-\frac{1}{p^s}} \tag{14}$$

is the Riemann zeta function, and

$$L(s) = \prod_p \frac{1}{1-\frac{1}{p^s}} \prod_r \frac{1}{1+\frac{1}{r^s}} \tag{15}$$

is an entire function of s [1].

The leading-order contribution to the $X \to \infty$ asymptotics of the integral (6) comes from the right-most pole of the integrand; this is the pole of $\zeta(s)$ at $s = 1$: $\zeta(s) = (s-1)^{-1} + O(1)$ as $s \to 1$. Thus

$$\sum_{n \le X} r_2(n) \sim X\frac{\pi}{4} \tag{16}$$

as $X \to \infty$, since [8]

$$L(1) = 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \ldots = \frac{\pi}{4}. \tag{17}$$

This clearly corresponds to the well-known asymptotics for the number of lattice points in a quarter circle. In the notation introduced above, it is equivalent to $M_1(N) \sim \pi/4$ as $N \to \infty$.

To quantify the error in the leading order asymptotics would require a calculation of the size of the integral along the contour deformed around the pole at $s = 1$, but we do not attempt that here. In specific cases, order estimates can be made (see, for example, [9]), however in general the true order is not known; even in the simple example just described, this is an viewed as an important unsolved problem [7].

It is also worth remarking that this error will depend on the type of averaging used to define the moments: if (7) is replaced by an infinite sum using a smooth characteristic function, the error will, in general, be reduced. The method described above then still applies, but with a modified integrand in (6). Again, since we are only concerned with the leading-order asymptotics, this further generalization will not be pursued here.

3 Second, third, and fourth moments

The generating function for the second moment is given by

$$\Xi_2(s) = \sum_{n=1}^{\infty} \frac{r_2^2(n)}{n^s} \tag{18}$$

$$= \frac{1}{1-\frac{1}{2^s}} \prod_r \frac{1}{1-\frac{1}{r^{2s}}} \prod_p \left[1 + \frac{4}{p^s} + \frac{9}{p^{2s}} + \ldots + \frac{(k+1)^2}{p^{ks}} + \ldots\right] . \tag{19}$$

As in the example of the last section, this can be checked by re-expanding the prime products, and then using (9). Performing the sum in the p-product gives

$$\Xi_2(s) = \frac{1}{1-\frac{1}{2^s}} \prod_r \frac{1}{1-\frac{1}{r^{2s}}} \prod_p \frac{1+\frac{1}{p^s}}{\left(1-\frac{1}{p^s}\right)^3} . \tag{20}$$

which can also be written in terms of $\zeta(s)$ and $L(s)$:

$$\Xi_2(s) = \frac{1}{\left(1+\frac{1}{2^s}\right)} \frac{\zeta^2(s)L^2(s)}{\zeta(2s)} . \tag{21}$$

Substituting this into (6), the right-most pole of the integrand is again the double pole of $\zeta^2(s)$ at $s = 1$ (the zeros of $\zeta(s)$ all have $\mathrm{Re}\, s < 1$ [9]). The leading order terms in the $N \to \infty$ asymptotics of the second moment then come from the residue at $s = 1$, and are

$$M_2(N) \sim \frac{1}{4} \log N + \alpha , \tag{22}$$

where, with primes denoting derivatives,

$$\alpha = \left(\frac{\gamma}{2} + \frac{2}{\pi} L'(1) - \frac{3}{\pi^2}\zeta'(2) + \frac{1}{12}\log 2 - \frac{1}{4}\right) , \tag{23}$$

which may be evaluated to give $\alpha \simeq 0.504$. The first term in (22) agrees with a calculation of Marklof [12] based on deep results from the theory of theta sums.

In numerical computations it is more convenient to use a local average for the moments,

$$\overline{r_2^k}(n) = \frac{1}{2W+1} \sum_{m=n-W}^{n+W} r_2^k(m) , \tag{24}$$

rather than (7). Then

$$\overline{r_2^2}(n) \sim \frac{d}{dn}\sum_{k=1}^{n} r_2^2(k) \sim \frac{1}{4}\log n + \alpha + \frac{1}{4} \tag{25}$$

as $n \to \infty$. In Figure 1 we plot this asymptotic approximation against $\log n$, together with a numerical computation of $\overline{r_2^2}(n)$ using (24) with $W = 250$ for $n \in \{251, 10000\}$ and $W = 500$ for $n \in \{10000, 19499\}$.

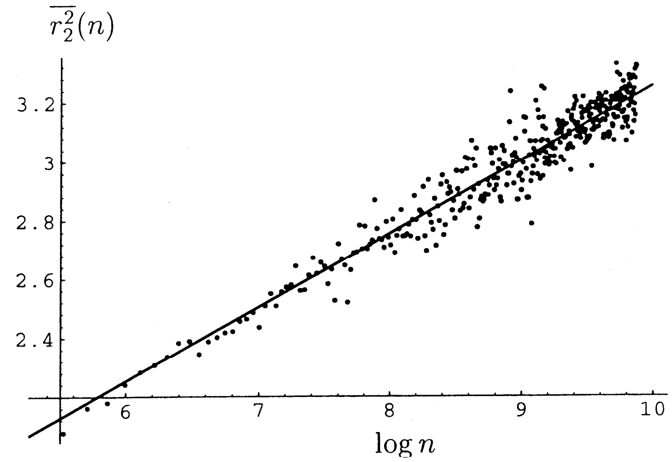

Figure 1: $\overline{r_2^2}(n)$ plotted against $\log n$. The dots are numerically computed values, the straight line represents the asymptotic approximation (25).

The generating function for the third moment of $r_2(n)$ is, in the same way, given by

$$\Xi_3(s) = \frac{1}{1-\frac{1}{2^s}}\prod_r \frac{1}{1-\frac{1}{r^{2s}}}\prod_p \left(1 + \frac{2^3}{p^s} + \frac{3^3}{p^{2s}} + \ldots + \frac{(m+1)^3}{p^{ms}} + \ldots\right). \tag{26}$$

The terms in the p-product sum to give

$$\Xi_3(s) = \frac{1}{1-\frac{1}{2^s}} \prod_r \frac{1}{1-\frac{1}{r^{2s}}} \prod_p \frac{1+\frac{4}{p^s}+\frac{1}{p^{2s}}}{\left(1-\frac{1}{p^s}\right)^4} \tag{27}$$

$$= [L(s)\zeta(s)]^4 \left(1-\frac{1}{2^s}\right)^3 \prod_r \left(1-\frac{1}{r^{2s}}\right)^3 \prod_p \left(1+\frac{4}{p^s}+\frac{1}{p^{2s}}\right)\left(1-\frac{1}{p^s}\right)^4$$

$$= [L(s)\zeta(s)]^4 B_3(s)\,, \tag{28}$$

where the last equality defines $B_3(s)$.

The reason for choosing this particular factorization is that $B_3(s)$ is singularity-free in the half-plane $\mathrm{Re}\, s \geq 1$; the r-product itself converges in this region, and the convergence of the p-product is guaranteed by the vanishing of the term proportional to $\frac{1}{p^s}$. The singularity that dominates the large-N asymptotics of the third moment is therefore again the pole of $\zeta(s)$ at $s = 1$.

Evaluating the resulting contribution to the integral in (6) then gives

$$
\begin{aligned}
M_3(N) \sim & \Big(\frac{\pi}{4}\Big)^4 \frac{1}{6} B_3(1) \log^3 N \\
& + \Big(\frac{\pi}{4}\Big)^4 \Big[\frac{1}{2} B_3'(1) + \Big(2\gamma - \frac{1}{2}\Big) B_3(1) + \frac{8}{\pi} B_3(1) L'(1)\Big] \log^2 N \\
& + \Big\{ \Big(\frac{\pi}{4}\Big)^4 \Big[\frac{1}{2} B_3''(1) + (1 - 4\gamma + 6\gamma^2 - 4\gamma(1)) B_3(1) + (4\gamma - 1) B_3'(1)\Big] \\
& \quad + \Big(\frac{\pi}{4}\Big)^3 \Big[16\gamma L'(1) B_3(1) + 4L'(1) B_3'(1) + 2B_3(1) L''(1) - 4B_3(1) L'(1)\Big] \\
& \quad + \Big(\frac{\pi}{4}\Big)^2 6B_3(1) [L'(1)]^2 \Big\} \log N \\
& + \Big\{ \Big(\frac{\pi}{4}\Big)^4 \Big[- 4B_3'(1)\gamma + 4B_3(1)\gamma^3 - B_3(1) + 2B_3(1)\gamma(2) + \frac{1}{6} B_3'''(1) \\
& \qquad + 6B_3'(1)\gamma^2 + 4B_3(1)\gamma(1) + 4B_3(1)\gamma - 6B_3(1)\gamma^2 - 4B_3'(1)\gamma(1) \\
& \qquad - \frac{1}{2} B_3''(1) - 12B_3(1)\gamma\gamma(1) + 2B_3''(1)\gamma + B_3'(1)\Big] \\
& + \Big(\frac{\pi}{4}\Big)^3 \Big[24B_3(1) L'(1)\gamma^2 - 4B_3'(1) L'(1) + \frac{2}{3} B_3(1) L'''(1) + 4B_3(1) L'(1) \\
& \qquad - 2B_3(1) L''(1) - 16B_3(1) L'(1)\gamma + 2B_3''(1) L'(1) \\
& \qquad - 16B_3(1) L'(1)\gamma(1) + 2B_3'(1) L''(1) + 8B_3(1)\gamma L''(1) \\
& \qquad + 16B_3'(1) L'(1)\gamma\Big] \\
& + \Big(\frac{\pi}{4}\Big)^2 \Big[6B_3(1) L'(1) L''(1) + 24B_3(1)\gamma [L'(1)]^2 + 6B_3'(1) [L'(1)]^2 \\
& \qquad - 6B_3(1) [L'(1)]^2\Big] + \Big(\frac{\pi}{4}\Big) 4B_3(1) [L'(1)]^3 \Big\}, \qquad (29)
\end{aligned}
$$

where primes again denote derivatives, $B_3(1) \simeq 0.0527$, $B_3'(1) \simeq 0.263$, $B_3''(1) \simeq 0.528$, $B_3'''(1) \simeq -1.521$, $L'(1) \simeq 0.193$, $L''(1) \simeq -0.153$ and $L'''(1) \simeq 0.0873$. The corresponding asymptotics for $\overline{r_2^3}(n) \sim \frac{d}{dn}(nM_3(n))$, obtained by substituting these values into (29), is plotted in Figure 2, together with data computed using (24) with $W = 10^3$ for $10^3 \le n < 10^6$ and $W = 10^5$ for $10^6 \le n < 10^{10}$.

It is worth remarking that the coefficient of the term that grows as $\log^3 n$ in $\overline{r_2^3}(n)$ is approximately 0.0033, the coefficient of the $\log^2 n$ term is approximately 0.0830, and the coefficient of the $\log n$ term is approximately 0.520.

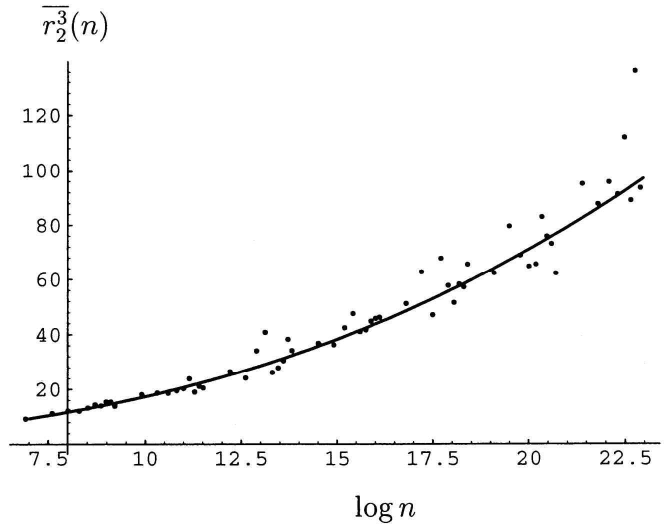

Figure 2: The asymptotic approximation for $\overline{r_2^3}(n)$, obtained from (29), and numerically computed values, plotted against $\log n$.

Thus while the first term dominates as $n \to \infty$, in the range of our numerical computations ($\log n < 23$) all are needed.

As a final explicit example, we now compute the leading-order term in the asymptotics of the fourth moment. The generating function in this case is

$$\Xi_4(s) = \frac{1}{1-\frac{1}{2^s}} \prod_r \frac{1}{1-\frac{1}{r^{2s}}} \prod_p \left(1 + \frac{2^4}{p^s} + \frac{3^4}{p^{2s}} + \ldots + \frac{(m+1)^4}{p^{ms}} + \ldots\right) \tag{30}$$

$$= \frac{1}{1-\frac{1}{2^s}} \prod_r \frac{1}{1-\frac{1}{r^{2s}}} \prod_p \frac{1 + \frac{11}{p^s} + \frac{11}{p^{2s}} + \frac{1}{p^{3s}}}{\left(1-\frac{1}{p^s}\right)^5} . \tag{31}$$

As above, we factorize this as

$$\Xi_4(s) = L^8(s)\zeta^8(s)B_4(s) , \tag{32}$$

where

$$B_4(s) = \left(1-\frac{1}{2^s}\right)^7 \prod_r \left(1-\frac{1}{r^{2s}}\right)^7 \prod_p \left(1+\frac{11}{p^s}+\frac{11}{p^{2s}}+\frac{1}{p^{3s}}\right)\left(1-\frac{1}{p^s}\right)^{11} \tag{33}$$

is, by virtue of the fact that there is no term proportional to $\frac{1}{p^s}$ in the p-product, singularity-free in $\operatorname{Re} s \geq 1$. Thus the right-most singularity is again that of $\zeta(s)$ at $s = 1$. Evaluating its contribution to the integral (6) then implies that to leading order in $\log N$ (that is, now neglecting terms that are $O(\log^6 N)$)

$$M_4(N) \sim \left(\frac{\pi}{4}\right)^8 \frac{B_4(1)}{5040} \log^7 N . \tag{34}$$

$\overline{r_2^4}(n)$ shares this same leading-order asymptotics.

Explicit expressions for the lower-order contributions can be written down in terms of the derivatives of $\zeta(s)$, $L(s)$ and $B_4(s)$, as before, but we do not present them here. Instead, we focus on the generalization of this leading-order result to all higher moments.

4 General moment asymptotics

Generalizing the scheme described above to k-th moment of $r_2(n)$ is straightforward. The generating function for $r_2^k(n)$ is

$$\Xi_k(s) = \frac{1}{1-\frac{1}{2^s}} \prod_r \frac{1}{1-\frac{1}{r^{2s}}} \prod_p \rho_k\left(\frac{1}{p^s}\right), \tag{35}$$

where

$$\rho_k(x) = 1 + 2^k x + 3^k x^2 + \ldots + (m+1)^k x^m + \ldots . \tag{36}$$

Thus from the examples considered in the previous section

$$\rho_0(x) = \frac{1}{1-x} \tag{37}$$

and

$$\rho_1(x) = \frac{1}{(1-x)^2} . \tag{38}$$

ρ_k satisfies

$$\rho_k(x) = \frac{d}{dx}\left[x\rho_{k-1}(x)\right] \tag{39}$$

and so we write

$$\rho_k(x) = \frac{1 + a_k x + b_k x^2 + \ldots}{(1-x)^{k+1}} . \tag{40}$$

Substituting (40) into (39) leads to a recurrence relation for a_k whose solution is

$$a_k = 2^k - k - 1 . \tag{41}$$

We now have that

$$\Xi_k(s) = \frac{1}{1-\frac{1}{2^s}} \prod_r \frac{1}{1-\frac{1}{r^{2s}}} \prod_p \frac{\left(1 + \frac{a_k}{p^s} + \frac{b_k}{p^{2s}} + \ldots\right)}{\left(1-\frac{1}{p^s}\right)^{k+1}} \tag{42}$$

$$= \frac{1}{1-\frac{1}{2^s}} \prod_r \frac{1}{1-\frac{1}{r^{2s}}} \prod_p \frac{1}{\left(1-\frac{1}{p^s}\right)^{k+1+a_k}} A_k(s) , \tag{43}$$

where

$$A_k(s) = \prod_p \left(1 + \frac{a_k}{p^s} + \frac{b_k}{p^{2s}} + \dots\right)\left(1 - \frac{1}{p^s}\right)^{a_k} \tag{44}$$

is, by construction (because it contains no term proportional to $\frac{1}{p^s}$) non-singular in $\mathrm{Re}\, s \geq 1$. It then follows from (41), and the fact that

$$\zeta(s)L(s) = \frac{1}{1-\frac{1}{2^s}} \prod_r \frac{1}{1-\frac{1}{r^{2s}}} \prod_p \frac{1}{\left(1-\frac{1}{p^s}\right)^2}, \tag{45}$$

that

$$\Xi_k(s) = [L(s)\zeta(s)]^{2^{k-1}} \times \left(1-\frac{1}{2^s}\right)^{2^{k-1}-1} \prod_r \left(1-\frac{1}{r^{2s}}\right)^{2^{k-1}-1} A_k(s) \tag{46}$$

$$= [L(s)\zeta(s)]^{2^{k-1}} B_k(s), \tag{47}$$

which defines $B_k(s)$.

When written in this way, the dominant contribution to the $X \to \infty$ asymptotics of the integral (6) comes from the pole of order 2^{k-1} at $s = 1$ associated with the zeta function. This then gives, to leading order in $\log N$,

$$M_k(N) \sim \frac{1}{(2^{k-1}-1)!} B_k(1) L(1)^{2^{k-1}} \log^{2^{k-1}-1} N, \tag{48}$$

the same formula also applying to $\overline{r_2^k(n)}$.

The asymptotic approximation (48) represents our main result. The divergence as $N \to \infty$ is due to the fact that the energy levels (1) of the square billiard are increasingly degenerate in the semiclassical limit. Our main purpose here was to draw attention to the strong dependence of the form of this divergence on the moment-power k. It is, of course, no surprise that higher moments are more sensitive to these degeneracies. What is surprising is the degree to which this is so. It suggests that the higher spectral moments may be worth studying in other systems whose levels have a limiting distribution that is non-Poissonian.

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