FLUCTUATIONS IN NUMBERS OF ENERGY LEVELS

M.V. Berry
University of Bristol

and

Research Center Bielefeld-Bochum-Stochastics
University of Bielefeld (FRG)

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by M.V.BERRY

In a recent paper (Berry 1985, hereinafter called I), I employed semiclassical techniques to obtain formulae for a particular statistic characterizing fluctuations of high-lying eigenvalues (excited energy levels) of quantal Hamiltonians. The statistic was the spectral rigidity $\Delta(L)$, defined for a set of levels $\{E_j\}$ in terms of the spectral staircase

$$\mathcal{N}(E) = \sum_{j=1} \Theta(E-E_j) \tag{1}$$

(Θ denotes the unit step function). $\Delta(L)$ is the least squares deviation of $\mathcal{N}(E)$ from a straight line over a stretch of L mean level spacings. My purpose here is to give a simplified outline of the rather difficult theoretical ideas developed in I, by applying them not to the rigidity but to a more elementary statistic, the <u>number variance</u> $\Sigma(L)$, which will now be defined.

A stretch of L mean level spacings, centred on energy E, extends from $E-L/2\langle d\rangle$ to $E+L/2\langle d\rangle$ where $\langle d\rangle$ is the mean level density

$$\langle d(E)\rangle \equiv \langle d\mathcal{N}(E)/dE\rangle. \tag{2}$$

Here and hereinafter, $\langle\ \rangle$ denotes semiclassical averaging, that is averaging over an energy range which is classically small but nevertheless large in comparison with h/T_{min} where T_{min} is the shortest classical orbit period (in the semiclassical limit $h\to 0$ this range contains many levels). The number of levels in this stretch is

$$n(L) = \mathcal{N}(E+L/2\langle d\rangle) - \mathcal{N}(E-L/2\langle d\rangle). \tag{3}$$

This fluctuates about the average value

$$\langle n(L)\rangle = L. \tag{4}$$

The number variance that we will calculate is the simplest measure of the size of the fluctuations:

$$\Sigma(L) \equiv \langle (n(L) - \langle n(L)\rangle)^2\rangle. \qquad (5)$$

On the basis of general spectral theory for ensembles of matrices (Bohigas and Giannoni 1984) we expect to understand the function $\Sigma(L)$ in terms of three universality classes. The first class is the Poisson spectrum of uncorrelated levels (arising from matrices factorizable into independent blocks), for which, of course

$$\Sigma_{\mathrm{poisson}}(L) = L \qquad (6)$$

The second class is the Gaussian orthogonal ensemble (GOE) of real symmetric matrices with random elements, for which

$$\Sigma_{\mathrm{GOE}}(L) \to \frac{2}{\pi^2}(\ell nL + \ell n2 + \gamma + 1 - \frac{\pi^2}{8}) \; (L \gg 1) \qquad (7)$$

where γ is Euler's constant 0.577... The third class is the Gaussian unitary ensemble (GUE) of complex Hermitian matrices with random elements, for which

$$\Sigma_{\mathrm{GUE}}(L) \to \frac{1}{\pi^2}(\ell nL + \ell n2 + \gamma + 1) \quad (L \gg 1) \qquad (8)$$

The aim is to derive these formulae not from random-matrix theory but from a semiclassical analysis based on the dynamics of the system (integrable or chaotic) as embodied in its classical closed orbits. The first main ingredient of the theory is the representation of the level density $d = d\mathcal{N}/dE$ as a sum over all distinct closed orbits at energy E (Gutzwiller 1978, Balian and Bloch 1972, Berry 1983, 1984):

$$d(E) = \langle d(E)\rangle + \sum_j A_j(E)\exp\{iS_j(E)/\hbar\}/\hbar^{1+\mu} \qquad (9)$$

In this formula, j denotes all closed orbits, including multiple traversals (negative - i.e. retracings - as well as positive). The (real) amplitudes A_j will be discussed later, when we come to the other main ingredients of the theory. S_j is the classical action round the j'th orbit (with possible focusing corrections not important here). The exponent μ is $\frac{1}{2}(N-1)$ for classically integrable systems with N freedoms (closed orbits forming (N-1) parameter families filling tori), and zero for chaotic ones (isolated unstable closed orbits). (The discussion here will be restricted to the integrable and chaotic extremes.)

We begin by applying (9) to the number of levels n(L) defined by (3), restricting L so that the range $L/\langle d\rangle$ remains classically small. (This allows L to be very large, because $\langle d\rangle \sim h^{-N}$ and if for example we demand $L/\langle d\rangle < \mathcal{O}(h^{1/2})$ we need only $L < \mathcal{O}(h^{-(N-1/2)})$.) Then, using $\partial S_j/\partial E = T_j$ where T_j is the j'th orbit period we get

$$n(L) = \int_{E-L/2\langle d\rangle}^{E+L/2\langle d\rangle} dE'\, d(E')$$

$$= L + \sum_j A_j \exp\{iS_j/\hbar\} \int_{-L/2\langle d\rangle}^{L/2\langle d\rangle} d\varepsilon\, \exp\{i\varepsilon T_j/\hbar\}/\hbar^{\mu+1}$$

$$= L + (2/\hbar^{\mu}) \sum_j (A_j/T_j) \exp\{iS_j/\hbar\} \sin\{LT_j/2\hbar\langle d\rangle\} \qquad (10)$$

To find the variance we square and use semiclassical averaging to eliminate uncompensated action exponentials. This gives

$$\Sigma(L) = \frac{4}{\hbar^{2\mu}} \left\langle \sum_i \sum_j \frac{A_j A_i}{T_j T_i} \exp\{\tfrac{i}{\hbar}(S_i - S_j)\} \sin\{\frac{LT_j}{2\hbar\langle d\rangle}\} \sin\{\frac{LT_i}{2\hbar\langle d\rangle}\} \right\rangle \qquad (11)$$

As explained in I, it is not always permissable to invoke semiclassical averaging to eliminate the off-diagonal terms in the sum, but it is correct to replace T_i and T_j by their average $(T_i+T_j)/2$. Thus

$$\Sigma(L) = \frac{8}{h^{2\mu}} \int_0^{\infty} dT\, \phi(T) \sin^2\{LT/2\hbar\langle d\rangle\}/T^2 \qquad (12)$$

where

$$\phi(T) \equiv \left\langle \sum_i \sum_j{}^{+} A_i A_j \exp\{i(S_i - S_j)/\hbar\}\, \delta\{T - (T_i + T_j)/2\} \right\rangle \qquad (13)$$

the + on the summation denoting restriction to positive traversals ($T_j > 0$). (In the corresponding formula for the rigidity $\Delta(L)$, $\sin^2$ in (12) is replaced by a more complicated function.)

The function $\phi(T)$ depends on the classical dynamics via the orbit action, periods and amplitudes. Provided $L \ll L_{max}$, where

$$L_{max} \equiv \hbar\langle d\rangle/T_{min} \sim h^{-(N-1)}, \qquad (14)$$

the integral in (12) depends on $\phi(T)$ for $T \gg T_{min}$, that is on <u>very long classical closed orbits.</u> (This exemplifies the general principle that spectral structure on a small energy scale ΔE depends on classical dynamics over long times $h/\Delta E$.) It is here that the second main ingredient enters the theory, in the form of classical sum rules obtained by Hannay and Ozorio de Almeida (1984) using the principle that very long orbits are uniformly distributed in phase space. Their sum rules concern the diagonal part ϕ_D of the sum (13), whose value results from two competing tendencies: The increasing density of orbits with period T (arising from the δ function factor) and their decreasing amplitudes A_j^2. They show that the result of this competition depends on classical dynamics, as follows:

$$\left.\begin{aligned}\phi_D(T) &\to \hbar^N \langle d\rangle/2\pi && \text{(integrable)}\\ &\to T/2\pi^2 && \text{(chaotic with time-reversal symmetry)}\\ &\to T/4\pi^2 && \text{(chaotic without time-reversal symmetry)}\end{aligned}\right\} \quad (\text{if } T \gg T_{min}) \qquad (15)$$

The factor 2 distinguishing $\phi_D(T)$ for chaotic systems with and without time-reversal symmetry has a very simple origin. With time--reversal symmetry, every closed orbit has a time-reversed counterpart with exactly the same action. These two orbits contribute coherently to the periodic orbit (9) and so their contribution to the squared function $\phi_D(T)$ is twice what it would be in the absence of this strict action degeneracy (i.e. $(A+A)^2=4A^2$ instead of the incoherent sum $A^2+A^2=2A^2$). This same factor 2 (and more generally, GOE rather than GUE statistics) will arise if the quantal Hamiltonian possesses any antiunitary symmetry, not necessarily time-reversal (Robnik and Berry 1985).

The three different T-dependences in (15) will lead to the three universality classes of variance (equations 6-8). It is necessary only to add the third main ingredient of the theory, which takes account of the fact that (13) cannot always be approximated by its diagonal part. The reason is that for very long times T, not just classically long but long in comparison with $\hbar\langle d\rangle \sim h^{-(N-1)}$, there can be pairs of distinct orbits with action differences S_i-S_j small in comparison with h, and these off-diagonal terms contribute coherently to (13). The third ingredient is a semiclassical sum rule (see I) giving $\phi(T)$ for such very long times and obtained from the condition that (9) must represent, asymptotically, a sequence of δ functions with the correct density $\langle d\rangle$. The rule is

$$\phi(T) \to \hbar^{2\mu+1}\langle d\rangle/2\pi \text{ if } T \gg h\langle d\rangle. \qquad (16)$$

It shows that the classical (diagonal) sum rule (15) adequately represents $\phi(T)$ only in the integrable case. For the two chaotic cases, (16) shows that the linear increase of $\phi_D(T)$ is eventully modified by the off-diagonal terms to give a $\phi(T)$ that saturates at a constant value.

Next it is convenient to define a scaled time

$$\tau \equiv T/2\pi\hbar\langle d\rangle, \tag{17}$$

and a scaled $\phi(T)$ by

$$K(\tau) \equiv 2\pi\phi(T)/\hbar^{2\mu+1}\langle d\rangle \tag{18}$$

Now the two sum rules (15) and (16) can be combined, to give

$$\left.\begin{array}{ll} K(\tau) \simeq 1 & \text{(integrable)} \\ K(\tau) \simeq 2\tau \text{ if } \tau\ll 1 \text{ and } 1 \text{ if } \tau\gg 1 & \text{(chaotic with time-reversal symmetry)} \\ K(\tau) \simeq \tau \text{ if } \tau\ll 1 \text{ and } 1 \text{ if } \tau\gg 1 & \text{(chaotic without time-reversal symmetry)} \end{array}\right\} \quad (\text{if } \tau\gg T_{min}/2\pi\hbar\langle d\rangle) \tag{19}$$

Physically, $K(\tau)$ is the <u>spectral form factor</u>: apart from a δ function at the origin,

$$K(\tau)=\langle d\rangle^{-2}\int_{-\infty}^{\infty}dL\ \langle d(E-L/2\langle d\rangle)d(E+L/2\langle d\rangle)\rangle\exp\{2\pi iL\tau\}. \tag{20}$$

In terms of K, the <u>pair correlation</u> of the levels is

$$g(L) = 1-\frac{1}{\pi L}\int_0^{\infty} d\tau\,\sin\{2\pi L\tau\}K'(\tau) \tag{21}$$

For integrable systems, (19) gives $g(L)=1$, that is an uncorrelated (Poisson) level sequence, as already established by Berry and Tabor (1977).

Using (17) and (18) we obtain from (12) the number variance

$$\Sigma(L) = \frac{2}{\pi^2}\int_0^{\infty}\frac{d\tau}{\tau^2}\,K(\tau)\,\sin^2\{\pi L\tau\}. \tag{22}$$

For $L\ll L_{max}$ (equation 14), we can evaluate this integral by substituting the formulae (19), because then Σ is determined by τ-values exceeding $T_{min}/2\pi\hbar\langle d\rangle$ and so depends only on the long closed orbits.

For <u>integrable systems</u>, substituting $K=1$ gives exactly $\Sigma=L$, i.e.

(6), and this is the first (Poisson) of the three universality classes. For chaotic systems without time-reversal symmetry, splitting the integration range at $\tau=u$ where $0<<u<<1$ leads to

$$\Sigma(L) = \frac{2}{\pi^2}\left[\ln L+\ln(2\pi)+\gamma-\frac{1}{2}\int_0^\infty d\tau \ln \frac{d}{d\tau}(K(\tau)/\tau)\right] \quad (L>>1) \tag{23}$$

which apart from the constant term is exactly the result (7) for the second (GOE) universality class. For chaotic systems without time-reversal symmetry the same technique gives

$$\Sigma(L) = \frac{1}{\pi^2}\left[\ln L+\ln(2\pi)+\gamma-\int_0^\infty d\tau \ln\tau \frac{d}{d\tau}(K(\tau)/\tau)\right] \quad (L>>1) \tag{24}$$

which apart from the constant term is exactly the result (8) for the third (GUE) universality class. The constant terms in (23) and (24) depend on how $K(\tau)$ interpolates between the linear and constant τ-regimes given by the two sum rules, and cannot be obtained by any semiclassical argument known to me (the constants are of order unity and so do not contribute to the leading-order asymptotics of $\Sigma(L)$).

This completes the main task, which was to explain the semiclassical origin of the three universal classes (6-8) of number variance. But it is important to point out that universality breaks down for correlations between distant levels, that is when $L\simeq L_{max}$. Then (19) cannot be employed because short times $T\sim T_{min}$ contribute to (12) and then $\Sigma(T)$ does not depend solely on the very long orbits. For $L>>L_{max}$, $\Sigma(L)$ saturates at the value

$$\Sigma_\infty = \frac{4}{\hbar^2\mu}\int_0^\infty dT\phi(T)/T^2 \tag{25}$$

For integrable systems, the diagonal sum for $\phi(T)$ gives Σ_∞ as a convergent sum over closed orbits:

$$\Sigma_\infty = \frac{4}{\hbar^{N-1}}\sum_j{}^{+} A_j^2/T_j^2 \tag{26}$$

For chaotic systems, extrapolation of the continuum results (24) gives the estimate

$$\left.\begin{aligned}&\Sigma_\infty \sim \frac{s}{\pi^2}\ln(\hbar\langle d\rangle/T_{min}\\ &\text{where } s=2 \text{ with time-reversal symmetry}\\ &\qquad\quad s=1 \text{ without time-reversal symmetry}\ .\end{aligned}\right\} \tag{27}$$

As discussed in I, a variety of numerical experiments support the theoretical ideas described here. In addition there have been two recent developments. Berry and Robnik (1985) have studied the change of spectral universality class when the time-reversal symmetry of particle motion in an enclosure with reflecting walls is broken by switching on a line of magnetic flux threading the enclosure ('Aharonov-Bohm quantum billiards'). And Seligman and Verbaarschot (1985) have studied spectral rigidity for motion in separable smooth potentials.

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