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Distribution of multiple avoided crossings: numerical evaluation

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Abstract. We compute numerically the distribution $\rho(\Delta\varepsilon)$ of $\Delta\varepsilon$, the local minimum distance (avoided crossing gap size) between neighbouring energy levels of two model systems We find that $\lim_{\Delta\varepsilon\to 0}\rho\sim\Delta\varepsilon$ The result differs from that expected for a GOE model, for which Wilkinson has shown that in the small $\Delta\varepsilon$ limit $\rho(\Delta\varepsilon)$ is constant We suggest that the discrepancy arises from parametric correlations which are known to exist but are absent from the GOE

When a classically chaotic Hamiltonian $H(\lambda)$, dependent on an external parameter λ, is solved quantum mechanically, the discrete spectrum $E_n(\lambda)$ has (generically) no degeneracies for any value of λ. There are instead near degeneracies, termed avoided crossings, which can be derived from degenerate perturbation theory [2]. As described in [1], in the (λ) neighbourhood of the near degeneracy, the two levels participating in the avoided crossing are effectively the two branches of a hyperbola.

More generally, the separation $S_n(\lambda)$ between neighbouring levels $E_n(\lambda)$ and $E_{n+1}(\lambda)$ will have local minima.

The subject of this paper is a numerical computation of the distribution of the sizes of these minima and a comparison with the theory of [1] for the sizes of avoided crossings. The models used are time reversal invariant and without spin, so their Hamiltonians are real symmetric matrices. This is also the case considered in detail in [1].

The complete description of what is to be calculated is the following. The spectrum $\{E_n(\lambda)\}$ is computed for the clasically chaotic Hamiltonian $H(\lambda)$. In general, the spectrum will not have a uniform local average density of states $\langle \mathrm{d}(E;\lambda)\rangle$ nor will the λ dependence of $\{E(\lambda)\}$ be linear. Both of these features introduce bias into any statistical measure on the spectrum, so it is necessary to normalize the spectrum by creating the unfolded spectrum $\{x_n(\lambda)\}$. One defines

$$N(E,\lambda)=\sum_{n=1}^{\infty}\Theta(E-E_n(\lambda)) \tag{1}$$

and its local average $\langle N(E;\lambda)\rangle$ satisfying

$$\frac{\partial\langle \mathrm{d}(E;\lambda)\rangle}{\partial E}=\langle N(E;\lambda)\rangle. \tag{2}$$

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The unfolded levels are then

$$x_n(\lambda) = \langle N(E_n(\lambda); \lambda) \rangle \approx n \tag{3}$$

for which the local average density of states is unity for all λ.

The separation S between levels is

$$S_n(\lambda) = x_{n+1}(\lambda) - x_n(\lambda) \tag{4}$$

and a local minimum occurs for an n_0 and λ_0 such that

$$\left.\frac{dS_{n_0}(\lambda)}{d\lambda}\right|_{\lambda=\lambda_0} = 0 \qquad \text{and} \qquad \left.\frac{d^2S_{n_0}(\lambda)}{d\lambda^2}\right|_{\lambda=\lambda_0} > 0. \tag{5}$$

The gap size of the local minimum is

$$\Delta\varepsilon_{n_0\,\lambda_0} = S_{n_0}(\lambda_0) \tag{6}$$

and from the set of all such local minima one produces the quantity of interest $\rho(\Delta\varepsilon)$, the distribution of local minima.

For small $\Delta\varepsilon$, the λ neighbourhood of the local minimum (avoided crossing) between levels n and $n+1$ can essentially be described by the 2×2 block of H, H_{ij}, $i, j \in \{n, n+1\}$. This matrix can be chosen to be diagonal for some arbitrary $\tilde{\lambda}$ in the neighbourhood and expanded to first order in λ elsewhere. As shown in [1], within the neighbourhood the levels form the two branches of a hyperbola whose five shape and position parameters are functions of the five parameters of the first order expansion. (These parameters are not the same as the parameter λ which will be called the physical parameter where confusion might arise.) Three of these are elements of the derivative matrix $(dH_{ij}/d\lambda)|_{\tilde{\lambda}}$. Thus, in order to derive a distribution of the shape parameters of the avoided crossings (including $\Delta\varepsilon$) the distribution of $dH/d\lambda$ is required.

In [1] Wilkinson takes this distribution to be GOE for the whole matrix and similarly the 2×2 block. That is

$$\left\langle \frac{dH_{ij}}{d\lambda} \right\rangle = 0 \tag{7}$$

and

$$\left\langle \left(\frac{dH_{ij}}{d\lambda} \right)^2 \right\rangle = (1+\delta_{ij})\sigma^2 \tag{8}$$

where $\langle\,\rangle$ is an ensemble average and σ is a constant.

H itself is also assumed to be GOE. While this is not exactly true for most completely chaotic Hamiltonians [3] it is correct for the level spacing distribution [4] which is what enters into the distribution of the shape parameters [1].

Wilkinson shows how these distributions lead to $\rho(\Delta\varepsilon)$ independent of $\Delta\varepsilon$ and confirms the result with computation on a model where both the Hamiltonian and its derivative are exactly members of the GOE. The model is built from white noise generated by a random number generator and as such does not have an immediate interpretation as a physical system

The goal of the present work is to evaluate $\rho(\Delta\varepsilon)$ for a physically meaningful model.

The major difficulty in a numerical evaluation of ρ is the need to work with a discrete set of λ values. Instead of $S_n(\lambda)$ as a continuous function of λ one has $S_n(\lambda' + l\delta\lambda)$, $0 \leq l \leq M-1$ where the spectrum of H has been evaluated for the M equally spaced λ values between λ' and $\lambda' + (M-1)\delta\lambda$.

Local minima are identified by the discrete version of condition (5). Writing $S_n(l)$ for $S_n(\lambda' + l\delta\lambda)$ this is

$$S_{n_0}(l_0-1) > S_{n_0}(l_0) < S_{n_0}(l_0+1). \tag{9}$$

It is necessary to ensure that the grid spacing is fine enough that all local minima are found.

The evaluation of $\Delta\varepsilon_{n_0,l_0}$ is done by quadratic interpolation through $S_{n_0}(l_0-1)$, $S_{n_0}(l_0)$ and $S_{n_0}(l_0+1)$. This is the most general leading order form of a local minimum. Checks on small minima (avoided crossings) showed that using a hyperbolic interpolation did not change the interpolated gap size significantly.

The distribution of local minima was computed for the two model systems considered in [5]. The first of these is the hydrogen atom in a uniform magnetic field. In cylindrical coordinates its Hamiltonian is

$$H = \frac{\bar{p}_r^2 + \bar{p}_z^2}{2} + \frac{\lambda^2}{8} r^2 - \frac{1}{\sqrt{r^2+z^2}} \tag{10}$$

which corresponds to the separable subspace $p_\varphi = 0$.

The spectrum and its unfolding were calculated according to [5] and references therein for the $M = 65$ partial spectra $\lambda' = 2.50 \times 10^{-5}$, $\delta\lambda = 1.25 \times 10^{-8}$ and $615 \leq n \leq 843$. A total of 919 local minima were identified.

The dots of figure 1 are the integrated distribution $F(\Delta\varepsilon)$

$$F(\Delta\varepsilon) = \int_0^{\Delta\varepsilon} \rho(t)\,\mathrm{d}t \tag{11}$$

calculated from the 919 local minima. The inset shows the behaviour for small $\Delta\varepsilon$.

According to the GOE model $F(\Delta\varepsilon)$ should grow linearly with $\Delta\varepsilon$ for small $\Delta\varepsilon$. This does not seem to be borne out by the data.

The 'true' distribution must go asymptotically to one for large $\Delta\varepsilon$ which suggests the *ansatz*

$$F(\Delta\varepsilon) = 1 - \mathrm{e}^{-\alpha\Delta\varepsilon} \tag{12}$$

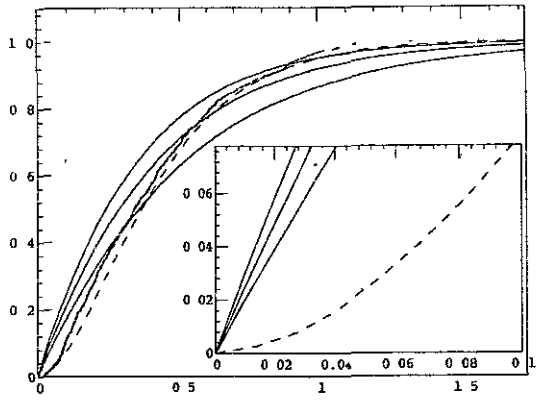

Figure 1. Integrated distribution of local minimum gap size $\Delta\varepsilon$ for the hydrogen atom in a magnetic field. Solid lines are *ansatz* (12) with $\alpha = 2, 2.5, 3$, dashed line *ansatz* (13) with $\beta = 4.71$. The inset shows the small $\Delta\varepsilon$ distribution

where α is a free parameter. The solid lines of figure 1 are *ansatz* (12) for the α values 2, 2.5 and 3, chosen to try and globally fit the data. There is no agreement with the small $\Delta\varepsilon$ values. While a small value of α would give a linear growth that would not be inconsistent with the small $\Delta\varepsilon$ values, the global form would be incorrect.

The data points of figure 1 indicate that $dF/d\Delta_\varepsilon$ vanishes at $\Delta\varepsilon = 0$. A different *ansatz* that reflects this is

$$F(\Delta\varepsilon) = 1 - (\beta\Delta\varepsilon + 1)\,e^{-\beta\Delta\varepsilon} \tag{13}$$

where β is a free parameter. The dashed line of figure 1 is (13) with $\beta = 4.71$. There is good agreement both globally and in the small $\Delta\varepsilon$ region.

Equation (13) corresponds to

$$\rho(\beta\Delta\varepsilon) = \beta\Delta\varepsilon\, e^{-\beta\Delta\varepsilon} \tag{14}$$

which is of Poisson form for large $\Delta\varepsilon$ but linear in $\Delta\varepsilon$ for small $\Delta\varepsilon$. This is physically reasonable because it means that when neighbouring levels are far apart they do not 'interact' strongly—local minima, or the fluctuations in the levels themselves, occur essentially randomly. Nearby levels, on the other hand, are correlated and 'repel' each other.

The second model system, also described in [5], is the 'Africa' billiard whose boundary is a conformal map of the unit circle ($z = e^{i\theta}$) from $\mathbb{C}$ to $\mathbb{C}$:

$$w = z + \frac{\cos\lambda}{\sqrt{10}}z^2 + \frac{\sin\lambda}{\sqrt{15}}e^{i\pi/3}z^3. \tag{15}$$

The Hamiltonian is infinite outside the boundary and the motion is free inside it.

Spectra and unfolding were calculated as in [5]. Here $M = 214$, $\lambda' = 0.14$, $\delta\lambda = 0.0016$ and $98 \leqslant n \leqslant 198$. A total of 716 local minima were identified

Figure 2 and its inset show $F(\Delta\varepsilon)$ calculated from these local minima. The solid line is *ansatz* (12) with $\alpha = 2.0$ and the broken line (13) with $\beta = 4.4$. The fluctuations are much stronger than in the first model, but the small $\Delta\varepsilon$ limit of F does not appear to be linear in $\Delta\varepsilon$.

The numerical results presented here seem to be in disagreement with the theory of [1]. Two possible sources of the discrepancy are the assumption that the local minima are well separated in parameter space so that they are independent, and that $dH/d\lambda$ is representative of a GOE.

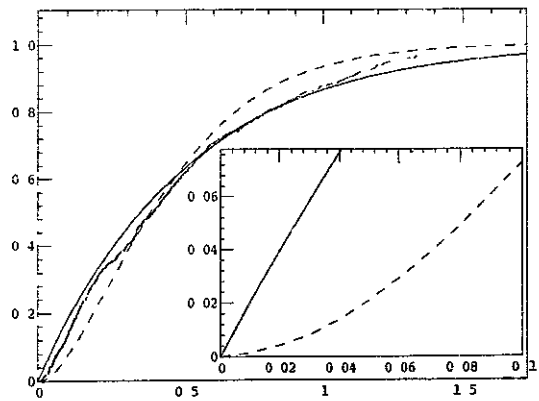

Figure 2. As figure 1 but for the Africa billiard Solid line $\alpha = 2$, dashed line $\beta = 4.40$.

A correlation distance for λ is provided by the parametric number variance [5]. For small λ displacements numerical evaluations agree with the semiclassical theory and spectra at nearby discrete λ values are correlated. For larger displacements correlation is lost and the parametric number variance saturates at twice Σ^2, the spectral number variance [4].

The independence of the local minima can be estimated by comparing the distribution $P(\Lambda)$ of displacements Λ between neighbouring local minima of $S_n(\lambda)$ with the parametric correlation distance. In figure 3 $P(\Lambda)$, the histogram, is plotted together with the numerical and semiclassical evaluations of the parametric number variance of the hydrogen plus magnetic field model. The correlation distance is approximately $\Lambda = 1.6 \times 10^{-7}$ and about 40% of the separations between local minima are less than this distance. Figure 4 is the same as figure 3 but for the Africa billiard. The parametric correlation distance is about $\Lambda = 0.22$ and some 85% of the separations are smaller

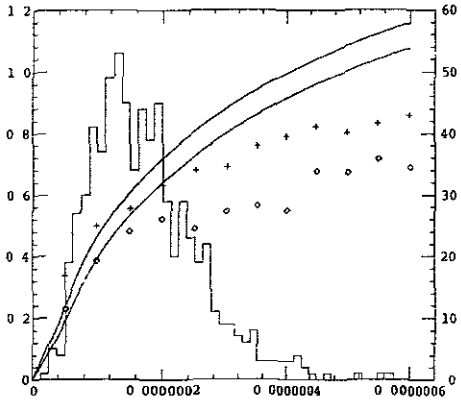

Figure 3. Distribution (histogram) of parameter distances between neighbouring local minima in the hydrogen atom plus magnetic field system. Crosses and diamonds, quantum computations of the parametric number variance. Solid lines, corresponding empirical fits of the semiclassical theory. Dotted line, semiclassical theory for the crosses determined solely from the classical dynamics. The correlation distance is approximately 1.6×10^{-7}

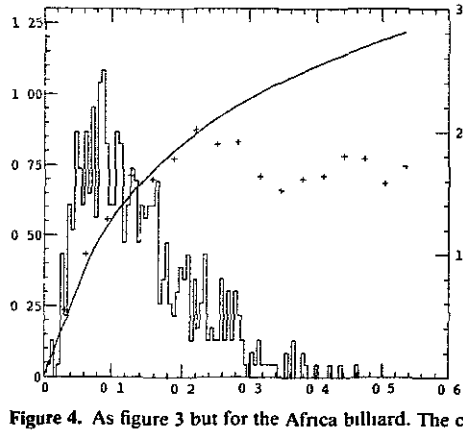

Figure 4. As figure 3 but for the Africa billiard. The correlation distance is approximately 0.22.

It should be remembered that each local minimum has two neighbouring minima, so that even in the hydrogen model the bulk of the local minima are closer than the correlation distance to another minimum. This suggests that the description of the local minima as independent hyperbolae is too crude.

The second assumption that may not hold is (8), that $dH/d\lambda$ in the diagonal basis of H is representative of a GOE. As pointed out in [1] if $dH/d\lambda$ is truly representative of a GOE then (8) will hold in any basis.

Evaluation of (8) involves performing the ensemble average, which corresponds to averaging over λ. For the first model,

$$\frac{dH}{d\lambda}=\frac{\lambda}{4}r^2. \tag{16}$$

The λ dependence is separable and the average over λ just gives a constant independent of the indices of the matrix element. The matrix elements of r^2 are products of radial integrals and angular integrals $I_a^{l,k}$ which are

$$I_a^{l,k}=\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta Y_l^0(\theta,\varphi)\, Y_k^0(\theta,\varphi)\sin^2\theta. \tag{17}$$

Standard angular momentum algebra shows that this integral vanishes unless $k=l, l\pm 2$ The fact that there are selection rules means that (8) cannot hold

A similar statement cannot be made about the Africa billiard since the λ dependence of H is not linear. The conformal form of (15) means that the free motion in Africa can be equivalently described as motion in a circular billiard with a position dependent mass. Writing $z=x+iy$, $|z|\leqslant 1$ as the coordinates inside the circle and w as in (15), the Hamiltonian inside the billiard is

$$H(x,y;\lambda)=\frac{1}{|\partial w(\lambda)/\partial z|^2}\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}\right). \tag{18}$$

When the derivative $dH/d\lambda$ is written explicitly it is easy to see that there is a complicated λ dependence and that there are no selection rules on the matrix elements.

An additional remark about parametric distributions can be made. The GOE model of [1] also predicts distributions for the other two shape parameters of the hyperbolae; the mean and difference between the slopes of the asymptotes. However, these distributions are strongly dependent on the choices of physical parameters There is no reason why the Hamiltonian cannot be described in terms of λ^2, $1/\lambda$ or any other reparametrization that preserves order in physical parameter space. It would seem that for the distribution of these other shape parameters to be invariant requires a strong (and so far unknown) ergodicity condition on the spectrum. Alternatively, a criterion such as uniformity in the positional distribution of local minima could be used to choose the parametrization in which statistics are to be measured. Such a criterion is implicit in much of the work on spectral statistics where averaging over different discrete, equally spaced λ values is assumed to involve uncorrelated spectra [4].

In summary, numerical evaluation of the distribution of the sizes of the local minima of the spacing between levels reveals that in two physical systems the small gap size distribution is not constant and is most probably quadratic in the gap size. This is in contrast to a GOE model of the distribution which predicts that the distribution is constant for small gap size.

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