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Nearest-neighbour spacing distribution of energy levels in the region between integrability and chaos

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Abstract. We derive an expression for the level spacing distribution for a quantal system displaying both regular and chaotic classical motion, assuming that the level-repulsion function for the mixed system is obtained by averaging the corresponding functions for the regular and chaotic regimes with weights given by their fractional phase-space volumes. The Liouville measures of the regular region obtained from comparing this expression with the level spacing distributions of a hydrogen atom in a uniform magnetic field agree with the corresponding values obtained in the classical-mechanical analysis of this system.

1. Introduction

It is generally agreed that the statistical properties of energy levels of a quantum-mechanical system whose classical counterpart is chaotic is well described by random matrix theory [1]. In the case in which there is anti-unitary symmetry, the nearest-neighbour spacing (NNS) distribution of energy levels of such a system is well approximated by a Wigner distribution:

$$P(s) = \tfrac{1}{2}\pi s \mathrm{e}^{-\pi s^2/4} \tag{1}$$

provided that the level sequence is normalized to unit mean level spacing. On the other hand, the NNS distribution of levels of a system whose classical dynamics is rigorous everywhere in the phase space is well represented by a Poisson distribution

$$P(s) = \mathrm{e}^{-s} \tag{2}$$

at least for not very large spacings. This conclusion is supported by several numerical experiments [2–4] as well as theoretical justifications based on semiclassical arguments [5, 6]. However, not all classical systems are either rigorous or chaotic. Computer studies of several non-integrable two-dimensional systems demonstrated that they undergo an order-to-chaos transition (see e.g. [7, 8]). Their classical phase space is mixed in the sense that some orbits wind regularly round two-dimensional tori and others explore the three-dimensional energy surface ergodically. In fact, the coexistence of regular and chaotic motion seems to be the general case, particularly in physical system. For example, while resonance spacings in neutron and proton scattering by atomic nuclei follow the Wigner distribution [9, 10], statistical tests of level spacings indicate transitional character between regular and chaotic regimes [11–13]. Other examples are provided by hydrogen atoms in strong magnetic fields [14], models of nuclear motion in simple molecules [15] and mesoscopic devices having a wide range of dynamical features [16].

The intermediate regime of mixed regular and chaotic dynamics is still a subject of intense research work. Various formulae have been proposed to fit the NNS distributions for mixed systems [17–21]. They depend on one parameter (or more), which can be tuned to interpolate between the limiting cases of regular and irregular spectra. The most popular of these formulae is the Brody distribution [17]:

$$P(s) = as^{\beta} \exp(-bs^{\beta+1}) \qquad a = (\beta+1)b \qquad b = [\Gamma((\beta+2)/(\beta+1))]^{\beta+1} \tag{3}$$

which assumes a power-law level repulsion and interpolates between the Poisson ($\beta = 0$) and Wigner ($\beta = 1$) distributions in a simple way.

A semiclassical theory for the level spacing of mixed systems has been given by Berry and Robnik [22] by assuming that the wavefunctions are localized in the ordered region of the phase space or in the chaotic regions. The energy levels then consist of separate sequences, one being Poisson distributed and each of the others being Wigner distributed. The relative weight of each distribution is given by the Liouville measure of the corresponding phase-space region. When this assumption holds, the NNS distribution in the case of a single chaotic region is given by

$$P(s) = \mathrm{e}^{-qs} \left\{ q^2 \,\mathrm{erfc}\left(\tfrac{1}{2}\sqrt{\pi}(1-q)s\right) + \left(2q(1-q) + \tfrac{1}{2}\pi(1-q)^3 s\right) \exp[-\tfrac{1}{4}\pi(1-q)^2 s^2] \right\} \tag{4}$$

where q is the measure of the regular region. Numerical experiments to date have resulted in NNS distributions [7, 8, 14, 21] consistent with (4) only for level spacings $s > 1$. Recently, Prosen and Robnik [23] have shown that the spectral superposition hypothesis certainly holds only in the deep semiclassical region. In an attempt to extend the validity of (4), they introduce the two-parameter 'ultimate' Berry–Robnik spacing distribution by describing the irregular levels (with measure $1 - q$) obey the Brody distribution with some β which is supposed to capture the localization of the underlying chaotic states. An extensive discussion for the effects leading to the departure form the semiclassical description of level statistics is given by Bohigas *et al* [24].

Hönig and Wintgen [21] presented numerical-experimental data of high statistical significance for the NNS distribution of the level spectra of the hydrogen atom in a uniform magnetic field. Their data included as small spacings as $s \approx 0.001$ and nevertheless the distributions did not show any tendency to vanish as s tended to zero as expected from Brody's formula, except in the cases of nearly chaotic spectra. Although the Berry–Robnik distribution (4) is the only one with a non-vanishing probability for very small spacings, their agreement with the data of [21] is very poor particularly in the region of $s < 1$. The best fits are obtained with the Brody formula (3) in spite of the fact that the analytic behaviour is incorrect near $s = 0$. In our view, this result is rather disappointing since the Brody interpolation parameter β does not have an explicit relation to the dynamics of the system.

In this paper, we propose an expression for the NNS distribution of the energy levels of a mixed system which depends on a single parameter and might be more suitable for comparison with experimental data. Our basic assumption is that the level-repulsion function for a mixed system can be taken as the average of the corresponding functions for the regular and chaotic systems with averaging weights equal to the measures of the phase-space domains of regular and chaotic motion, respectively. We find that the values of these measures obtained from the analysis of spectral fluctuations of the paramagnetic hydrogen atom [21] are in good agreement with the corresponding values obtained in the classical analysis.

The NNS distribution of levels of unit mean spacing can be derived [25] from a simple probability argument, which results in the following integral equation:

$$P(s) = r(s) \int_s^\infty P(x)\,\mathrm{d}x \tag{5}$$

where $r(s)$ is the level-repulsion function defined so that $r(s)\,\mathrm{d}s$ is the conditional probability that, given a level at energy E, there is one level in the interval $\mathrm{d}s$ provided that there are no levels in the interval $(E, E+s)$. This equation can be solved by first converting it into a differential equation which can then be integrated to obtain

$$P(s) = r(s) \exp\left[-\int_0^s r(x)\,\mathrm{d}x\right] \tag{6}$$

where the lower integration limit in the exponent is set equal to zero to make $P(s) \simeq r(s)$ for small values of s. The cumulative spacing distribution is then given by

$$W(s) = \int_0^s P(x)\,\mathrm{d}x = 1 - \exp\left[-\int_0^s r(x)\,\mathrm{d}x\right]. \tag{7}$$

The Poisson distribution (2) can be obtained from (6) by taking

$$r_{\mathrm{Poisson}}(s) = 1 \tag{8}$$

which is consistent with the fact that, in the regular regime, the conditional probability density of finding a level in a given spacing interval does not depend on the length of this interval. On the other hand, the Wigner formula (1) for the NNS distribution of levels of a time-reversal-invariant chaotic system is obtained by the following choice of the level-repulsion function:

$$r_{\mathrm{Wigner}}(s) = \tfrac{1}{2}\pi s \tag{9}$$

where the constant factor ensures a unit average level spacing.

Berry [26] has suggested the following derivation of (9). Consider an ensemble of real Hamiltonians $H(\boldsymbol{R})$ smoothly parametrized by a set of parameters $\boldsymbol{R} = (R_1, R_2, \ldots)$. Suppose that at some point $\boldsymbol{R}'$ of the parameter space two states $|1'\rangle$ and $|2'\rangle$ are degenerate with energy $E' = E$, i.e.

$$H(\boldsymbol{R}')|1'\rangle = E'|1'\rangle \qquad \text{and} \qquad H(\boldsymbol{R}')|2'\rangle = E'|2'\rangle. \tag{10}$$

If $\boldsymbol{R}'$ is slightly varied into $\boldsymbol{R}$, according to the degenerate perturbation theory, the energy splits to the first order in $\boldsymbol{R} - \boldsymbol{R}'$ by

$$\Delta E(\boldsymbol{R}) = [\{H'_{11}(\boldsymbol{R}) - \boldsymbol{H}'_{22}(\boldsymbol{R})\}^2 + 4H'^2_{12}(\boldsymbol{R})]^{1/2} \tag{11}$$

where

$$H'_{ij} = \langle i'|H(\boldsymbol{R}) - H(\boldsymbol{R}')|j'\rangle. \tag{12}$$

At a degeneracy $\Delta E = 0$, which implies the following two independent conditions on the matrix elements of H:

$$H'_{11}(\boldsymbol{R}) = H_{22}(\boldsymbol{R}) \qquad \text{and} \qquad H'_{12}(\boldsymbol{R}) = 0. \tag{13}$$

These conditions can be satisfied only if the Hamiltonian depends on at least $n = 2$ parameters. For a system with parameters $\boldsymbol{R}$ with NNS defined so as to have an average value unity, the Nth spacing is given by

$$s_N = [E_{N+1}(\boldsymbol{R}) - E_N(\boldsymbol{R})]\frac{\mathrm{d}N(E_N, \boldsymbol{R})}{\mathrm{d}E_N} \tag{14}$$

where $N(E, \boldsymbol{R})$ denotes the smooth number of levels below E. Berry assumes ergodicity to replace the energy average by ensemble averaging (over parameters R). The NNS distribution is then defined as

$$P(s) = \langle \delta(s - s_N(\boldsymbol{R}) \rangle_R \tag{15}$$

where $\langle\rangle_R$ denotes ensemble averaging. The cumulative spacing distribution, defined by the integration of $P(s)$ from 0 to s, will then be equal to the volume of the fraction of the parameter space in which $s_N(\boldsymbol{R}) \leqslant s$. Thus, for small values of s,

$$\int_0^s P(x)\,\mathrm{d}x \propto s^2 \tag{16}$$

which implies that, as $s \to 0$,

$$P(s) \cong r(s) \propto s. \tag{17}$$

Berry's parameter-space method has also been applied to describe systems without time-reversal symmetry [26]. These systems have to be described by an ensemble of Hermitian Hamiltonians having complex non-diagonal matrix elements. Equations (13) will then impose three conditions. The corresponding parameter space will be at least three-dimensional and the level-repulsion function will be quadratic. The same arguments can also be used to describe regular systems. In this case, small perturbations do not remove degeneracies and conditions (13) do not apply so that an ensemble of one-parameter Hamiltonians can be used to describe a regular system. However, we cannot see any way to use similar arguments to obtain a level-repulsion function proportional to a non-integer power of s as required to obtain Brody's interpolation formula (3).

In order to apply Berry's method to mixed system, we recall the representation of the transition from integrability to chaos in terms of the Poincaré surfaces of section, e.g. in the case of a hydrogen atom in a uniform magnetic field [14]. In the absence of the magnetic field the motion is confined to tori and the surface of section will simply give continuous loops representing quasiperiodic rotational and vibrational motion. Introducing a weak field does not change the surface of section although the motion is, strictly speaking, not confined to tori. Indeed, tori having a rational winding number are replaced, even under an infinitesimal perturbation, by a stable n-cycle embedded in a stochastic layer. However, the widths of the layers are infinitesimally small and hence invisible near the integrable limit. As we increase the scaled energy (see (21) below) irregular motion first appears near the separatrix transforming it into a stochastic layer. As we further increase the scaled energy, this layer increases in size whereas the large islands related to regular motion become smaller and finally almost disappear. We try to apply the previous scenario to the stochastic transition of a bound quantum system. The energy spectrum of a regular quantum system has the property of level clustering. We may expect that, in general, introducing a weak perturbation does not change this property, although, strictly speaking, any infinitesimal perturbation will result in removing the degeneracies. However, the shifts in the energy levels are infinitesimally small and hence invisible near the integrable limit. As we increase the perturbation, the level shift will increase but by different amounts in different parts of the spectrum. We now follow Percival's semiclassical classification of states of a bound quantum system into regular and chaotic classes, each related in some sense to the corresponding domain in the classical phase space [27]. We assume that the two classes have different feelings for the perturbation; the integrable class will keep the property of level clustering (within a resolution defined, e.g., by the width of the step of the NNS distribution histogram) while the chaotic states will be non-degenerate. In other words, if the wavefunction of a regular state is expanded in terms of the eigenstates of the integrable term of the Hamiltonian, only one (of very few) of the expansion coefficients will have a significant magnitude. On the other hand, the chaotic states will be delocalized in the unperturbed basis [20]. This picture can be justified by referring to the shell-model calculation carried out by Meridith *et al* [28] using the three-orbital Lipkin–Meshkov–Glick model [29]. These authors calculated the distribution functions for the overlap coefficients of the eigenfunctions of the model with a set of basis. For a typical member of the Gaussian orthogonal ensemble (GOE), the overlap is a Gaussian random variable [25]. For an integrable system, the distribution has a few very large overlaps and many very small overlaps (in keeping with the normalization condition). The resulting overlap distributions for all dynamical classes in the transitional region between regularity and chaos showed the same qualitative behaviour: an excess of very small overlaps and very large overlaps relative to a Gaussian distribution. This finding may be interpreted as indication for the coexistence of almost-regular and almost-chaotic states in a system in the integrability-chaos transition regime.

Berry's parameter-space description can now be introduced by assuming that the mixed system can be described by a combination of two ensembles. The first is an ensemble of one-parameter Hamiltonians which describes the regular states while the second is an ensemble of Hamiltonians depending on two parameters at least. The number of members of each ensemble is proportional to the corresponding classical phase-space volume. Following arguments similar to those leading to (17), we obtain

$$r(s) = q r_{\mathrm{Poisson}}(s) + (1-q) r_{\mathrm{Wigner}}(s) \tag{18}$$

where q is the fractional volume of the regular phase-space domain. Substituting (8), (9) and (18) into (6), we finally obtain

$$P(s) = [q + \tfrac{1}{2}\pi(1-q)s]\exp[-qs - \tfrac{1}{4}\pi(1-q)s^2]. \tag{19}$$

We hope that this expression will be useful for the analysis of the NNS distribution of the energy levels of natural mixed systems such as hydrogen atoms in magnetic fields and nuclei at low excitation energies, for which $P(s) \neq 0$. It does not vanish at $s = 0$ as Brody's formula. It interpolates in a simple way between the Wigner ($q = 0$) and the Poisson distributions. It has a similar behaviour at large s as the Berry–Robnik formula (4). Moreover, it yields $P(0) = q$ which is smaller than the value of $P(0) = q(2-q)$ obtained from (4). Therefore, it will probably be more capable of producing the minimum at small spacings of the NNS distributions observed for systems with intermediate values of q.

We note that the assumption (18) leads to a value of the mean spacing slightly larger than unity when $q \neq 0$ or 1. It is thus necessary to normalize the energy scale to ensure that the mean level spacing is unity. Replacing s by ε/D and defining D by requiring that $\int_0^\infty sP(s)\,\mathrm{d}s = 1$, we obtain

$$\frac{1}{D} = \frac{\exp(a^2)}{\sqrt{1-q^2}}\,\mathrm{erfc}(a) \qquad a = q\Big/\sqrt{\pi(1-q)}. \tag{20}$$

Using (20), we find that D starts from a value of 1 at $q = 0$, increases with increasing q, reaches a maximum value of 1.06 at $q = 0.67$ and then decreases and returns to the value 1 at $q = 1$. We thus conclude that the normalization of the energy scale in equation (19) does not lead to appreciable modification of the NNS distribution.

2. Comparison with numerical experiment

Wintgen and collaborators [14, 21, 28] carried out a detailed study of the classical- and quantum-mechanical properties of the hydrogen atom in a uniform magnetic field. The classical dynamics of this system does not depend on energy E or magnetic field strength γ (expressed in atomic units) separately, but depends only on the scaled energy

$$\varepsilon = E\gamma^{-2/3}. \tag{21}$$

These authors showed by calculating the Poincaré surfaces of section that the classical system displayed a smooth transition from regularity to chaos as the parameter ε increased from -0.8 to -0.1. Then, they solved the Schrödinger equation for fixed values of the scaled energy ε and obtained a large-scale spectrum for each value. The total number of levels in a case varied from 2980 for $\varepsilon = -0.10$ to 12 800 for $\varepsilon = -0.40$. The high statistical significance of these data invited us to use them to check the quality of the NNS distribution proposed in the previous section.

The cumulative spacing distribution obtained by integrating (19) from 0 to s takes a particularly simple form:

$$W(s) = 1 - \exp[-qs - \tfrac{1}{4}\pi(1-q)s^2]. \tag{22}$$

In particular, the quantity $\ln[1-W(s)]$ becomes a linear expression in q when $W(s)$ is given by (22). We calculated q for each point of the cumulative spacing distributions reported in [21] and took the average for each of these distributions. Table 1 lists the average values of q, with their standard deviations taken as measures of errors, for seven values of the scaled energy. The corresponding values q_{cl} of the fractional volume of the domain of regular motion of the classical phase space are also given in table 1. The table shows that the estimates for the measure of the classical phase-space domain of regular motion, obtained from the analysis of the cumulative spacing distributions, are in good agreement with the corresponding values obtained in the classical analysis. An exception is the case of $\varepsilon = -0.3$ which does not show the typical dependence of the distributions on the scaled energy, as pointed out by Hönig and Wintgen [21].

Table 1. Fractional volume q_{cl} of the regular classical phase space and q values obtained by fitting cumulative spacing distribution to (22) together with q_{BR} obtained in [30] by fitting the NNS distribution to the Berry–Robnik formula (4).

ε	q_{cl}	q	q_{BR}
-0.10	0.00	0.02 ± 0.02	0.00
-0.15	0.04	0.03 ± 0.02	
-0.20	0.12	0.08 ± 0.02	0.09
-0.25	0.16	0.20 ± 0.03	
-0.30	0.24	0.14 ± 0.03	0.35
-0.35	0.40	0.37 ± 0.08	
-0.40	0.66	0.58 ± 0.09	0.60

Figure 1 shows a comparison between the cumulative distributions calculated by means of (22) with those of the numerical experiment [21]. The agreement between the two sets of distributions is quite satisfactory, noting that the curves are represented in a logarithmic scale. Exceptions are in the region of spacings in which $W(s) < 10^{-3}$ where the results of the numerical experiment are of less statistical significance. Figure 2 compares the NNS distributions calculated using (19) and these are shown as full curves, with the histograms of the level spacings of a hydrogen atom in a magnetic field given in [28] and the predictions of the Berry–Robnik formula shown as dotted curves. It is clear from the figure that the proposed formula for the level-distribution provided a good representation for the histogram again except for the case of $\varepsilon = -0.30$ which does not conform to the general trend. It gives a better description of the numerical experiment than the Berry–Robnik formula in the region of small spacings, otherwise the two formulae are almost equivalent.

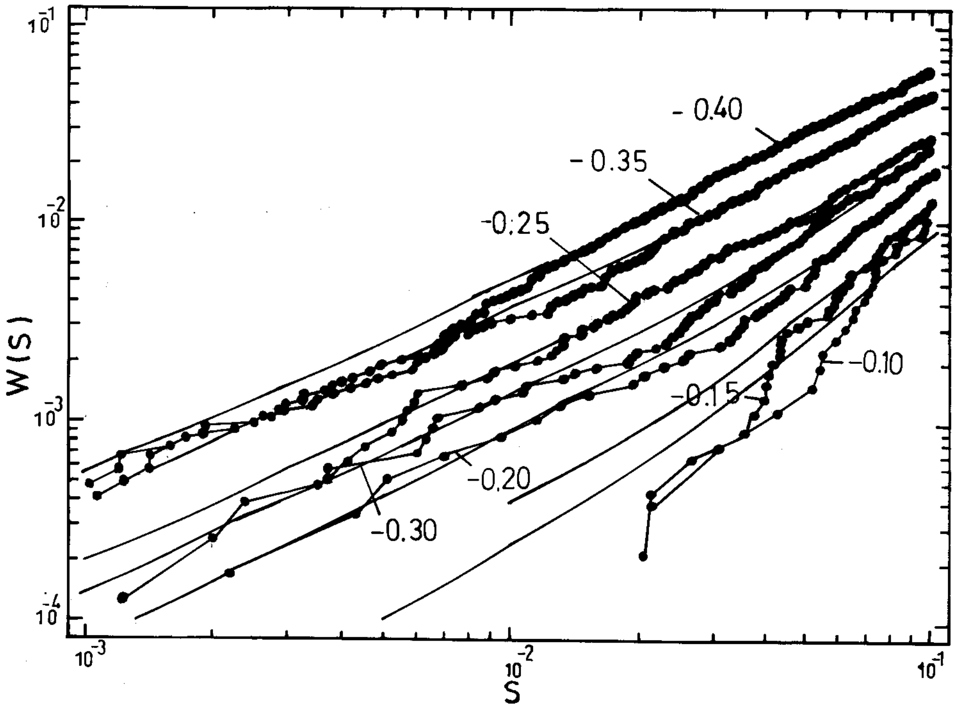

Figure 1. Comparison between the cumulative spacing distributions calculated from (22) and those reported in [21].

3. Summary and conclusions

We have obtained a simple expression for the NNS distribution of the energy levels of a quantum system whose classical dynamics is a mixture of regular and chaotic motion. It contains one parameter, which is assumed to be equal to the fractional volume $q_{\rm cl}$ of the regular domain of the classical phase space of the system. The derivation of this expression is based on Percival's classification scheme that separates the eigenstates into regular and chaotic groups. Each group is described by an ensemble of Hamiltonians in their parameter space. Following the arguments suggested by Berry leads to a level-repulsion function, which coincides with the NNS distribution at small spacings, as a superposition of two terms describing the two types of dynamics and having weights given by the corresponding volumes of the classical phase space.

We have compared the proposed expressions for the NNS distribution (equation (19)) and the cumulative spacing distribution (equation (22)) with the numerical calculations of the energy levels of a hydrogen atom in a uniform magnetic field reported by Wintgen *et al*. The results of the comparison, shown in figures 1 and 2, suggest that these expressions provide a reasonable description of the level distribution. In particular, the predictions of (19) are in agreement with those of the Berry–Robnik formula at $s > 1$ but provide a better description of the numerical experiment at small spacings. Perhaps the most important

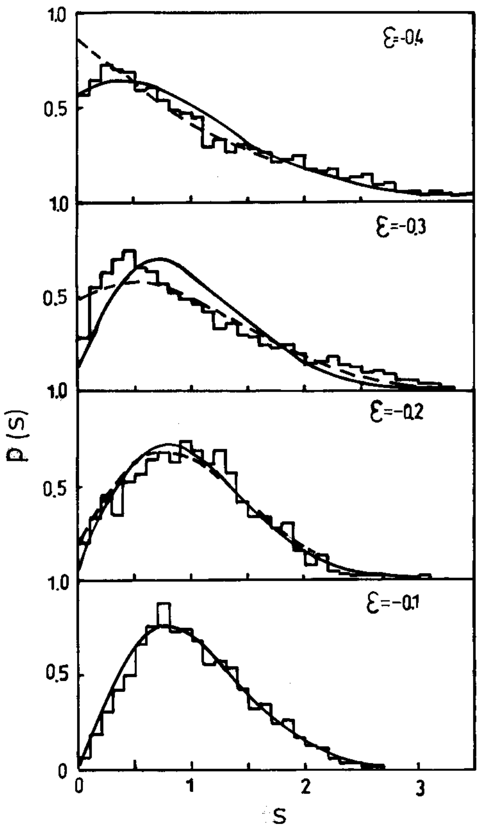

Figure 2. Comparison between the NNS distributions calculated from (19) and represented by full curves with those reported in [30] where the histograms are the results of the numerical experiment and the dotted curves are the predictions of the Berry–Robnik formula (4).

conclusion which can be drawn from this comparison is the close agreement between the values of the fractional phase-space volume of the domain of regular motion extracted from the analysis of spectra and the corresponding values obtained from the classical-mechanical analysis.

We finally note the proposed formula does not apply to the specific quantum chaotic systems recently considered by Zakrewski *et al* [31]. Among these systems is the hydrogen atom in a magnetic field (along the z-axis) near the ionization threshold. In this case, the electron can explore the region in the phase space very far of the nucleus where the Coulomb potential $1/\sqrt{\rho^2+z^2} \cong 1/|z|$, leading to an adiabatic separation of motion along the $\rho-$ and z-coordinates. Then, the coupling between various n_z Rydberg series associated with different n_ρ may not be strong enough to mix the various series and allow the occurrence of chaotic states.

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