PHYSICAL REVIEW A VOLUME 38, NUMBER 1 JULY 1, 1988

Stochastic formulation of energy-level statistics

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(Received 29 June 1987; revised manuscript received 29 January 1988)

It is shown that the joint distribution of energy eigenvalues for systems with a varying degree of nonintegrability which has been obtained dynamically by T. Yukawa [Phys. Rev. Lett. **54**, 1883 (1985)] can also be deduced by putting his equations of motion in the form of stochastic differential equations. We obtain an interpolation formula for the nearest-neighbor-spacing distribution as a smooth one-parameter family of density functions $P_\lambda(S)$, $0 \leq \lambda < \infty$. This distribution retains a nonanalytic nature near $\lambda \rightarrow 0$; when $\lambda = 0$ it agrees with the Poissonian distribution but whenever $\lambda \neq 0$ it is proportional to S for small S, as predicted by M. Robnik [J. Phys. A **20**, L495 (1987)]. A considerable improvement on the agreement between the energy-level histogram in a real system (hydrogen in a magnetic field) and theoretical formulas which have been studied by Wintgen and Friedrich [Phys. Rev. A **35**, 1464 (1987)] is demonstrated.

There has been growing interest in energy-level statistics for quantum systems with Hamiltonians which lie in the intermediate regime of transition from integrability to chaos.[1] A convenient way to describe the statistics for such systems presently adopted by many authors is to compute energy levels from secular determinants of very high dimension and to plot the frequency histogram of the nearest-neighbor level spacings (NNS), which may be compared with theoretical predictions [two well-known limiting distributions, Poisson-type and Gaussian-orthogonal-ensemble (GOE) type (or Wigner type), have so far been used]. For example, the quantum spectrum of the hydrogen atom in static magnetic fields of laboratory strength is regarded as an ideal system for this study[2] both theoretically and experimentally, where the diamagnetic effects allow one to see the development of quantum chaos. Another example is a driven quantum system such as the driven anisotropic spin, where a transition from regular to irregular behavior is found in the quasienergy spectrum with increasing strength of the driving magnetic field.[3]

The theoretical prediction for the statistics in such a controllable situation seems unestablished to date. The first explicit evidence that the proposed interpolation formula due to Berry and Robnik[1] is inadequate for guiding the actual frequency histogram has been reported by Wintgen and Friedrich[2] in their study of the hydrogen-atom levels in a magnetic field. Robnik[4] has accordingly discussed the reason for this inadequacy, proposing some examples of improvement. Our specific aim here is to provide an explicit answer to the question raised by these two recent works.

We report a result which is motivated by recent work of Yukawa.[5] Our approach is to transform his dynamical equations of motion into stochastic ones, which allows us to find the distribution by means of the standard theory of Brownian motion and stochastic differential equations. Thus the stationary solution of a relevant Fokker-Planck equation will give the distribution. This is an approach basically suggested in Dyson's paper in 1962 (Ref. 6) and reformulated recently by Tanaka and Sugano.[7] These treatments, however, are only to give the joint distribution of a Gaussian ensemble without discussing how the degree of regularity can be taken into account. Here we wish to note the importance of distinguishing the problem of obtaining the NNS distribution from that of justifying the joint distribution in the random-matrix theory. We begin with the latter problem along the line of making Yukawa's equation of motion stochastic before proceeding to the NNS problem.

Let $H_t = H_0 + tV$ be an $N \times N$ real, symmetry Hamiltonian matrix represented on a certain fixed orthogonal basis [we confine ourselves to the GOE case—a discussion about the Gaussian unitary ensemble (GUE) is given later], where H_0 is the Hamiltonian of a regular system and tV a perturbation with strength t which is regarded as the time variable in the dynamics under study (Dyson's fictitious time). On converting to the diagonal representation of H_t with eigenvalues labeled as $[x_1(t), x_2(t), \ldots]$ all assumed nondegenerate, Yukawa obtained the two sets of equations of motion

$$\dot{x}_n = p_n, \quad \dot{p}_n = 2 \sum_{n'(\neq n)} \frac{f_{nn'}^2}{(x_n - x_n')^3}, \quad n = 1, 2, \ldots, N \tag{1}$$

and a third set giving $\dot{f}_{nm}$ in terms of $\{x_n\}$ and $\{f_{nm}, n \neq m\}$ which close the equations for the full system described by N canonical pairs $\{x_n, p_n\}_{n=1}^N$ together with additional $\frac{1}{2}N(N-1)$ variables $\{f_{nm}\}$ that are noncanonical. Then it follows that this dynamical system is a completely integrable one.[5,8] It is worth noting that in this virtual dynamics the canonical momentum p_n conjugate to the eigenvalue x_n is given by V_{nn}, and the other variables $f_{nm}(n \neq m)$ related to V_{nm}, by

$$f_{nm}=(x_n-x_m)V_{nm} , \tag{2}$$

i.e., the diagonal and off-diagonal elements of the perturbation V, respectively, with respect to the exact eigenvectors of the H_t. Among a number of possible constants of motion which exist owing to the complete integrability, Yukawa chooses two specific forms, namely, the energy

$$K=\frac{1}{2}\sum_{n=1}^{N} p_n^2+\frac{1}{2}\sum_{\substack{n,m\\(n\neq m)}} \frac{f_{nm}^2}{(x_n-x_m)^2}$$

and the angular momentum

$$Q=\frac{1}{2}\sum_{\substack{n,m\\(n\neq m)}} f_{nm}^2 ,$$

in the "canonical equilibrium distribution" $e^{-\beta K-\gamma Q}$, and integrates the latter over all irrelevant variables $\{p_n\}$ and $\{f_{nm}\}$ to obtain the density of the joint distribution for $\{x_n\}$ as follows:

$$P(x_1,\ldots,x_N)=C_N\prod_{\substack{n,m\\(n>m)}}\left[\frac{(x_n-x_m)^2}{1+(\gamma/\beta)(x_n-x_m)^2}\right]^{1/2} \tag{3}$$

$$\simeq C\prod_{\substack{n,m\\(n>m)}}|x_n-x_m|\exp\left[-\frac{N\gamma}{2\beta}\sum_{(n)}(x_n-\bar{x})^2\right],\quad \bar{x}=\frac{1}{N}\sum_{(n=1)}^{N}x_n , \tag{3'}$$

where Eq. (3'), nothing but the joint GOE distribution from the random-matrix theory, is deduced in the limit $\gamma[\sim O(N^{-1})]\rightarrow 0$. Yukawa implies that Eq. (3) yields the intermediate situation between the chaotic and regular limits in terms of the ratio γ/β, when varied in the range $(0,\infty)$. We aim to find the NNS distribution formula in such situations by a stochastic reformulation of Yukawa's Eq. (1).

Let us first replace (1) by a set of Langevin equations,

$$\dot{x}_n=p_n ,$$
$$\dot{p}_n=-\Gamma p_n+\sum_{n'(\neq n)}\frac{2V_{nn'}^2}{x_n-x_{n'}}+R_n(t) , \tag{1'}$$
$$\Gamma>0$$

with a friction constant Γ and external noise forces $R_n(t)$ of Gaussian white character. The friction constant Γ is related to the strength σ of the Gaussian white noise $R_n(t)$ as $\sigma^2=2\beta^{-1}\Gamma$ (this assures the equipartition value β^{-1} of p_n^2 as $t\rightarrow\infty$). The set of equations for $\{x_n,p_n\}$ is then analogous to that for the Ornstein-Uhlenbeck Brownian motion, which may reduce to the Smoluchowsky type with the momentum p_n being dropped from the process, provided a coarse graining of the time scale is assumed (that is to say, the dynamics is described on a time scale much coarser than Γ^{-1}). A simple but correct way of performing this is to put $\dot{p}_n=0$ and to insert the resulting p_n from the last equation into the first one $\dot{x}_n=p_n$ ("adiabatic elimination"). This gives

$$\dot{x}_n=\frac{1}{\Gamma}\left[\sum_{n'(\neq n)}\frac{2V_{nn'}^2}{x_n-x_{n'}}+R_n(t)\right] . \tag{4}$$

It is a many-body Langevin equation which appears equivalent to Dyson's formulation of the Brownian motions of the eigenvalues [his Smoluchowski equation (19) (Ref. 6) with friction constant f which is identified to our Γ]. We find that the averaging procedure for $V_{nn'}^2$, in the above equation adopted by Dyson, only provides the prefactor

$$\prod_{(n>m)}(x_n-x_m)$$

of the GOE limit distribution (3'), and hence it must be replaced by a more relevant treatment.

Combining any pair of (4), we replace it by the equation of motion for $x_{nm}=x_n-x_m$ as

$$\dot{x}_{nm}=\frac{1}{\Gamma}\left[\sum_{n'(\neq n,m)}\left[\frac{2V_{nn'}^2}{x_{nn'}}+\frac{2V_{mn'}^2}{x_{n'm}}\right]+R_{nm}\right]+\frac{4V_{nm}^2}{\Gamma x_{nm}} . \tag{4'}$$

Our method of treating this equation can be stated as follows.

(i) All the unknown quantities $V_{nn'}$'s are regarded as independent, Gaussian random variables each of which tends to a white noise in the limit $N\rightarrow\infty$.

(ii) As a starting approximation to the many-body character of the equation, Eq. (4') is simplified as a single equation for $x_{nm}(n>m)$ by absorbing $x_{nn'}$ (or $x_{n'm}$) of the denominator into the random variable of the respective numerator, except that the variable x_{nm} of the *same* pair is retained as in the last part of (4') (this appears as a process-dependent noise force which is essential for the level-repulsion effect).

The approximation (ii) implies that the correlations between different spacings are ignored to zeroth order and hence all $x_{nm}(n>m)$'s are statistically independent.

The treatment of process-dependent noise forces in the theory of Brownian motion requires special care, because it gives rise to the problem of how to define the multiplication rule of the process and the white noise. Following the fact that the white limit of a sequence of nonwhite noises yields the symmetrized product (so called "Stratonovich product"),[9] we now write our stochastic differential equation (SDE) for x_{nm} as follows:

$$dx_{nm}(t)=\sigma d\hat{B}_{nm}(t)+\frac{\lambda}{x_{nm}(t)}\circ dB_{nm}(t) . \tag{5}$$

Here $\hat{B}_{nm}(t)$ and $B_{nm}(t)$ are two orthogonal standard Brownian motions [the orthogonality can be seen from their respective sources, i.e., the weighted sum of $V^2_{n(m),n'}$ over $n'(\neq n,m)$ for the former and the single term V^2_{nm} for the latter], σ and λ are constants to represent the strength of the respective Brownian motion, and the symbol $\circ$ implies the symmetrized product of $x_{nm}(t)^{-1}$ and $dB_{nm}(t)$. It is then possible to study the process $x_{nm}(t)$ and its distribution using the standard theory of SDE,[10] in particular, subjected to the rule of transformation between the Stratonovich SDE and the Itô SDE (the so-called stochastic calculus[11]).

The stationary distribution of the process $x_{nm}(t)$ subject to the SDE (5) is determined by the stationary solution of the associated Fokker-Planck equation. We will show that this is of the form

$$\{x^2_{nm}/[1+(\sigma/\lambda)^2x^2_{nm}]\}^{1/2} .$$

Hence by virtue of the statistical independence of all the processes $x_{nm}(t)$, $n>m$, the joint probability density for the eigenvalues $x_n(t)$ is identical to (3), if

$$\gamma/\beta=(\sigma/\lambda)^2 . \tag{6}$$

This allows an interpretation of Yukawa's parameters β and γ as being related to two different kinds of fluctuations, $B(t)$ and $\hat{B}(t)$: β $[\lambda B(t)]$ represents the fluctuations associated with the level-repulsion effect, whereas γ $[\sigma\hat{B}(t)]$ represents all other fluctuations.

In order to assure that Eq. (5) as SDE yields a stationary distribution of the above-stated form, we give here a more general result about a specific class of SDE. We consider a one-dimensional SDE of the form

$$dx_t=\sum_{(i=1)}^{r} b_i(x_t)\circ dB^{(i)}(t) , \tag{7}$$

where $b_i(x)$ is a smooth function of the variable x, and r real Brownian motions $\{B^{(i)}(t)\}$ satisfy the standard correlation properties $E\,dB^{(i)}(t)dB^{(j)}(t)=\delta_{ij}dt$. Then, the Fokker-Planck equation for the probability density $P_t(x)$ of the process x_t, defined by means of the conditional expectation of the diffusion processes:

$$E[f(x_t)\,|\,x_{t=0}=x]=\int f(x)P_t(x)dx$$

is given by

$$\frac{\partial}{\partial t}P_t(x)=\frac{\partial}{\partial x}\left[P_t(x)\left[\tfrac{1}{2}D'(x)+D(x)\frac{\partial}{\partial x}\log P_t(x)\right]\right] \tag{8}$$

with

$$D(x)=\tfrac{1}{2}\sum_{(i=1)}^{r} b_i(x)^2 ,$$
$$D'(x)=\frac{d}{dx}D(x) . \tag{9}$$

The stationary solution of Eq. (8) is obtained, in the generic cases, from

$$\tfrac{1}{2}D'(x)+D(x)\frac{d}{dt}\log P(x)=0$$

which yields

$$P(x)=N[2D(x)]^{-1/2}=\frac{N}{\left[\sum_{(i=1)}^{r} b_i(x)^2\right]^{1/2}} . \tag{10}$$

The solution to Eq. (5) follows from this general result for $r=2$, $b_1=\sigma$, $b_2=\lambda/x_{nm}$. The formal analysis to ascertain this result is to compute the drift velocity and the diffusion coefficient $D(x)$ of the solution process x_t of (7), for which two expressions in (9) give the answer. Note that for such a process with nonconstant diffusion coefficient special care is necessary for dealing with the drift velocity, and each symmetrized product $b_i(x_t)\circ dB^{(i)}(t)$ of the defining SDE (7) yields the contribution $-\frac{1}{2}b_i(x)b_i'(x)$ to the total drift (to be summed up by virtue of $E\,dB^{(i)}dB^{(j)}=0$, $i\neq j$) when the diffusion operator is written in the symmetrized form as in (8); a fact which can be deduced by the Stratonovich-Itô transformation, a general prediction being $Y\circ dX=Y\,dX+\frac{1}{2}dY\,dX$ in the stochastic calculus.[11,12] To be mathematically rigorous about the above result it is necessary to specify the boundary condition for the diffusion process x_t, which is beyond the present analysis: In fact, Yukawa's distribution (3) by itself is unnormalizable in the whole space, and we might introduce a conventional convergence factor to avoid the difficulty so that we replace the constant σ by $\sigma e^{\epsilon x}$ ($\epsilon>0$) and then let ϵ tend to zero in converting from (3) to (3'). This concludes an outline of the stochastic derivation of Yukawa's result.

As an application, we now wish to derive an explicit interpolation formula for the NNS distribution which may replace the two familiar ones so far used,[1] the one due to Brody and the other due to Berry and Robnik. In order to do this we must restrict (5) to pairs (n,m) which represent a nearest-neighbor spacing, and we would have to account for many-body correlation effects which force the pair (n,m) to be an NNS. To avoid the complexity of a rigorous procedure we assume that all such effects can be lumped together in an appropriate dependence of the two noise-strength parameters σ and λ on the NNS variable $S=x_{nm}$. These functions $\sigma(S)$ and $\lambda(S)$ can be determined in the two limiting situations by exploiting a known result about the statistics for NNS: Namely, if $\mu(x)$ denotes a level density, the expression $\exp-\int_0^S\mu(x)dx$ represents the conditional probability that the open interval $(0,S)$ is empty of levels if 0 is occupied by one level. Typically one has $\mu(x)=\text{const}(=\rho)$ for the Poissonian and $\mu(x)=\text{const}(=\bar{\rho})x$ for the Wigner surmise.[12] When $\lambda=0$, the desired SDE must yield the Poissonian stationary distribution and can be derived by replacing $dx_{nm}(t)$ in (5) by $e^{-\rho S_t}\circ dS_t$, thus

$$dS_t=\sigma e^{\rho S_t}\circ d\hat{B}(t),\ \text{i.e.},\ \sigma(S)=\sigma e^{\rho S}\ . \tag{11}$$

Similarly, when $\sigma=0$, the SDE with the Wigner surmise as the stationary distribution is given by

$$dS_t=\frac{\lambda}{S_t}e^{(1/2)\bar{\rho}^2 S_t^2}\circ dB(t),\ \text{i.e.},\ \lambda(S)=\frac{\lambda}{S}e^{\bar{\rho}^2 S^2}\ . \tag{12}$$

In each case the average level density ρ or $\bar{\rho}$ is determined from the scaling normalization, i.e., $\langle S\rangle$ $[=\int P(S)S\,dS]=1$ to give $\rho=1$ for the Poissonian and $\bar{\rho}=(\pi/2)^{1/2}$ for the Wigner surmise, but for the intermediate purpose they may play the role of parameters.

To bridge both limits for such intermediate situations we thus make an ansatz by writing the SDE as the sum of the two types of noises in (11) and (12):

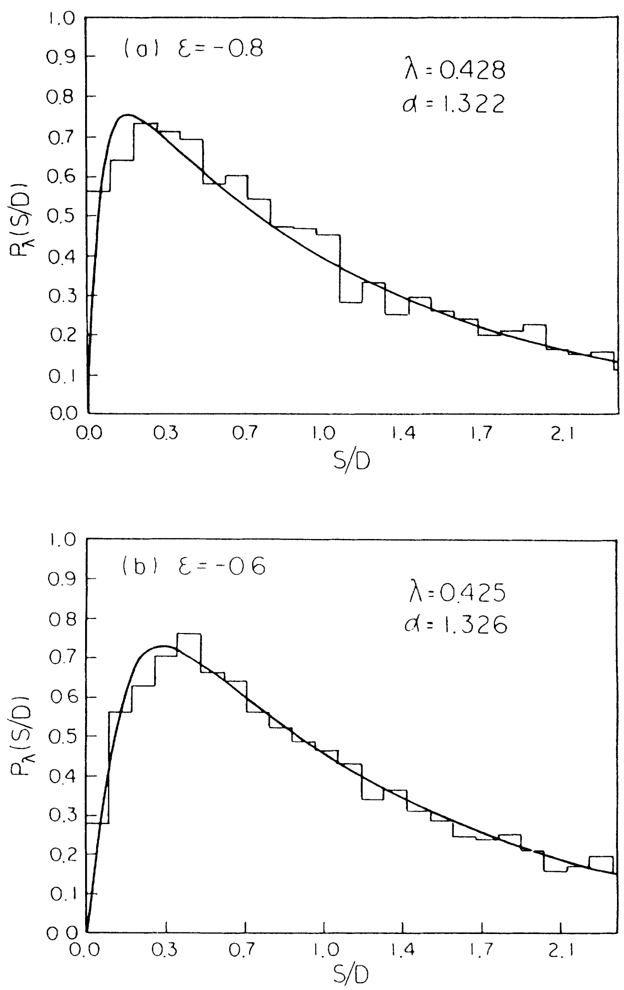

FIG. 1. A least-square fit of the nearest-neighbor spacing histogram computed by Wintgen and Friedrich in Fig. 2 of Ref. 2 [Phys. Rev. A **35**, 1464 (1987)] to the formula (14). The computation was made by Wunner. The scaling unit D is unity in the formula (14), and the scaled energy ϵ is equal to $B^{-2/3}E$ in terms of the magnetic field strength B and the actual energy E.

$$dS_t=\sigma e^{\rho S_t}\circ d\hat{B}(t)+\frac{\lambda}{S_t}e^{(\alpha^2/2)\rho^2 S_t^2}\circ dB(t)\ , \tag{13}$$

with

$$\alpha=\bar{\rho}/\rho\ . \tag{13a}$$

Then, we can apply the result (10) for the stated class of SDE (7) to get

$$P_\lambda(S)=\frac{N\rho S e^{-\rho S-(\alpha^2/2)\rho^2 s^2}}{(\rho^2 S^2 e^{-\alpha^2\rho^2 S^2}+\lambda^2 e^{-2\rho S})^{1/2}},\quad 0\le S<\infty \tag{14}$$

where the constant σ has been absorbed into the normalization factor N and into a renormalization of the strength λ of the repulsive noise $dB(t)$. The third constant α is left free to represent a characteristic of individual systems. The normalization $\langle 1\rangle=1$ and the scaling normalization $\langle S\rangle=1$ [which can be performed analytically by the use of (14) (Ref. 13)] will determine N and ρ as functions of λ and α. If one plots this simple interpolation formula for values of the nonintegrability parameter λ varying from 0 to infinity (the other parameter α being fixed), one gets a smooth one-parameter family of curves which satisfies the aspect of the NNS distribution to be anticipated,[13] in particular, the universality near $S=0$ discussed by Robnik.[4] Namely, in the absence of level repulsion (i.e., $\lambda=0$) $P_\lambda(S)$ reduces to the Poissonian, but its presence, no matter how small, makes $P_\lambda(S)$ proportional to S for $S<\lambda$. This nonanalytic nature is just what Robnik argues to be universal for all those nearly regular systems which tend to characteristic of GOE distribution in the chaotic limit, and not equipped with in the Berry-Robnik as well as Brody formulas. On the other hand, the allowance of the third parameter α makes the present formula not universal in the whole range of λ, which also conforms to his argument.

In spite of the lack of such a global universality, Robnik[4] argued the existence of a family of $P(S)$ which shows an overall good fit to the NNS histogram in many cases. He proposed an expression for $P(S)$ from the principle of *maximum entropy* under the constraint $\langle S^2\rangle=$prescribed (besides $\langle 1\rangle=\langle S\rangle=1$), which corresponds essentially to our formula (14) with the square-root denominator being omitted. (We note, however, that the underlying variational principle to deduce this result is not the principle of maximum entropy but rather the principle of minimum entropy production for the stationary solution of a Fokker-Planck equation.[14]) Thus, the result (14) provides an answer in favor of his ansatz. More precisely, the ansatz can be regarded as ideally satisfied if the extra parameter α in (14) appears insensitive to the nonintegrability parameter λ for an individual system. In Fig. 1 a comparison of the formula (14) is made with the NNS histogram of Wintgen and Friedrich computed for the hydrogen atom in a magnetic field in the transition regime,[2] and one sees an excellent fit to remedy the deficiency of the Berry-Robnik formula. It would be interesting to study further the role of the parameter α in developing the chaos.

Finally, we remark about the possibility of extending the present approach to the case of GUS: the applicability of the equation-of-motion method to the energy-level statistics in GUS was first mentioned by Yukawa[4] and then discussed in detail by Robnik[15] with an emphasis of distinction between the absence and presence of an extra antiunitary symmetry (the latter situation yields the GOE). It is hoped to obtain a satisfactory extension, but so far an adequate form of SDE has not been found.

We thank G. Wunner for providing us with important information and K. Nakamura for a motivation for the formulation. One of us (H.H.) acknowledges M. Toda, P. Davis, and S. Adachi for useful comments and Deutscher Akademischer Austauschdient for financial support.

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