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Nonuniversality in Curvature Distributions of Quantum Levels

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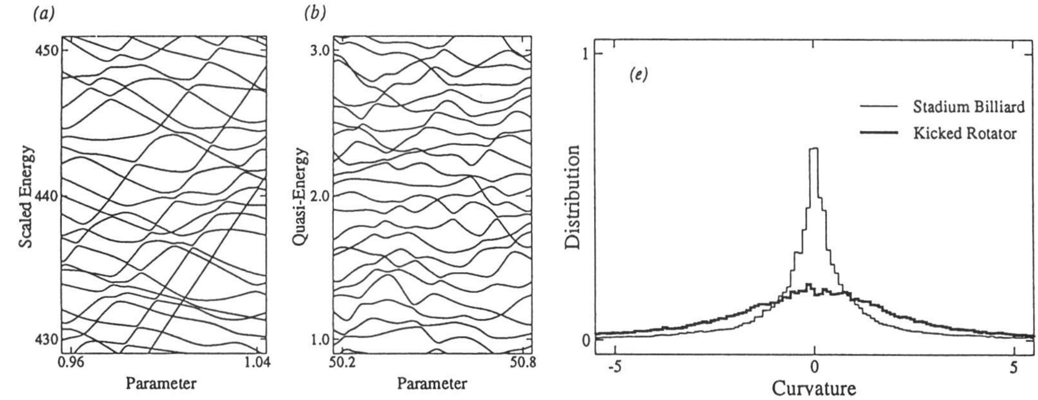
We are motivated by the recent theoretical analyses of Zakrzewski and Delande(Z-D) on curverture distribution of chaotic quantum levels to construct a unified theory which is capable of predicting the nonuniversal feature of the distribution $P(K)$: while $P(K)$ for large values of the curverture K of an irregular quantum level, embedded in a level diagram moving as a parametric motion with λ (i.e. $K = \frac{d^2E}{d\lambda^2}$), has the universal power law $P(K) \sim K^{-(\nu+2)}$, $P(K)$ for $K \approx 0$ is different for different individual systems with variety of sharpened peaks, as we have demonstrated previously. We utilize the stochastic freqency modulation theory of Kubo who formulated the motional narrowing of resonant line shape in the context of Gaussian stochastic processes. Thus, a satisfactory scheme of interpolating the two limiting forms of $P(K)$ proposed by Z-D has been achieved.

1. Introduction

Our previous numerical investigation of the curvature distributions of complex quantum levels moving according to a change of an adiabatic parameter (Takami and Hasegawa[1)]) revealed that, although the distribution (density function) $P_{curv}(K)$ for large K values behaves like $K^{-(\nu+2)}$, $\nu = 1$ for GOE and $\nu = 2$ for GUE, in agreement with the theoretical prediction of universality due to a level-dynamical formulation by Gaspard et al[2)], its peak behavior around $K = 0$ differs greatly from one sample to another chosen in the numerical tests (see Fig.1). This feature about nonuniversality has been one of the major clarifying points of the recent theoretical analyses on the parametric motion of chaotic quantum levels contained in two papers by Zakrzewski and Delande[3)] (in abbreviation Z-D hereafter) and Zakrzewski et al[4)]. See also the preceding review in this volume[5)].

In this report we discuss a probabilistic formulation of the curvature distribution of levels for a fully chaotic quantum system, where the origin of the two formulas for $P_{curv}(K)$ proposed in Z-D will be clarified in terms of the "relative correlation length in the parameter" of



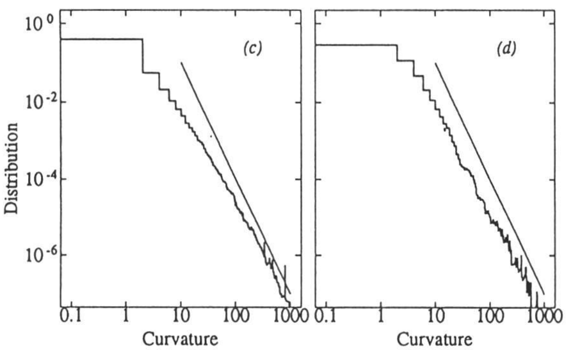


Figure 1: Parametric motion of eigenvalues: (a) stadium billiard; (b) kicked rotator, and numerically obtained histograms of the curvature distributions: (c) stadium billiard; (d) kicked rotator; (e) comparison of the small curvature behavior between the stadium billiard (thin line) and the kicked rotator (thick line).

random influence acting on the pair of moving levels: The first formula (eq. (4.15) in Z–D, constructed as a two-level statistical model of the level dynamics) reads

$$P_{\text{curv}}(K) = C_\nu K^{\frac{\nu-2}{2}} \mathcal{D}_{-\frac{3}{2}\nu-1}(B_\nu K) \tag{1}$$

with normalization and scaling constants C_ν and B_ν, and in terms of the parabolic–cylindrical related function

$$\mathcal{D}_{-p}(z) \equiv \frac{1}{\Gamma(p)} \int_0^\infty e^{-\frac{t^2}{2}-zt} t^{p-1} dt.$$

It corresponds to the shortest (zero) limits of the correlation length, implying that the level dynamics of the pair is taking place as if it were unaffected by any other levels. For GOE ($\nu = 1$), the formula yields a sharpened peak of $P_{\text{curv}}(K)$ at $K = 0$.

On the other hand, the second formula (eq. (3.27) in Z–D, proposed just intuitively) which reads

$$P_{\text{curv}}(K) = N_\nu (1 + B'^2_\nu K^2)^{-\frac{\nu+2}{2}} \tag{2}$$

with normalization N_ν, and another scaling constant B'_ν, is a consequence of the Gaussian stochastic assumption on the influence of all other levels than the pair, in the case of very long correlation length. Note also that the Wigner type function is assumed for the spacing distribution in both (1) and (2) (see below).

Our theoretical basis to deduce the above results is Kubo's stochastic frequency modulation theory[6] plus the so-called generalized Langevin method[6]: His concept of 'motional narrowing' is incorporated in the short-correlation formula (1). Numerical interpolation between the two limiting situations (1) and (2) will be exhibited.

2. Probabilistic Formulation

First, we point out that the curvature distribution $P_{curv}(K)$ can be expressed reasonably as an integral transform of the spacing distribution for an adjacent pair of levels $P_{sp}(s)$ such that

$$P_{curv}(K) = \int_{-\infty}^{\infty} F(K,s) P_{sp}(s) ds. \tag{3}$$

Here, we may assume the symmetry property

$$P_{curv}(-K) = P_{curv}(K),\ P_{sp}(-s) = P_{sp}(s),\ \textit{and hence}\ F(-K, \pm s) = F(K,s). \tag{4}$$

The probabilistic meaning assigned to the kernel function $F(K,s)$ represents the conditional curvature distribution associated to any pair of levels x_1 and x_2 under the condition that these are neighboring and have the spacing value s i.e.

$$x_2(\lambda) - x_1(\lambda) = s, \tag{5}$$

where the curvature K associated to (x_1, x_2) is defined by

$$K \equiv \frac{d^2}{d\lambda^2} \frac{1}{2}(x_2(\lambda) - x_1(\lambda)). \tag{6}$$

We can show the correctness of the expression (3) with the additional assignment (5) and (6) along the line of statistical mechanical formulation by Gaspard et al (unrestricted to the tail part, however) [2], which should be presented elsewhere.

Our key tool for presenting the result stated in Section 1 is to investigate the characteristic function (i.e. the Fourier transform) of the distribution/conditional distribution, namely

$$\Phi(t) \equiv \int_{-\infty}^{\infty} P_{\mathsf{curv}}(K)\ e^{iKt} dK = 2 \int_{0}^{\infty} \Phi(t,s) P_{\mathsf{sp}}(s) ds \tag{7}$$

$$\Phi(t,s) \equiv \int_{-\infty}^{\infty} F(K,s)\ e^{iKt} dK. \tag{8}$$

Then, the most important finding of Gaspard et al[2], namely the universal tail behavior of the curvature distribution $P_{\mathsf{curv}}(K)$ can be transcribed by some simple scaling properties of $F(K,s)$ and its characteristic function $\Phi(t,s)$ as follows: Suppose that the spacing distribution $P_{\mathsf{sp}}(s)$ assumes the power form $A_\nu s^\nu + O(s^{\nu+1})$ for small s values. The scaling property for F,

$$F(K,s) = |K|^{-1} f(Ks) \quad \text{such that} \quad \int_0^{\infty} f(k) k^\mu dk < \infty, \quad \mu \leq -1, \tag{9}$$

or, that for Φ

$$\Phi(t,s) = \phi(\frac{t}{s}) \quad \text{such that} \quad \int_0^\infty |\frac{d^{\mu+1}}{dt^{\mu+1}}\phi(t)|dt < \infty \tag{10}$$

assures the universal tail behavior of $P_{\text{curv}}(K)$ as

$$P_{\text{curv}}(K) \overset{|K|\to\infty}{\longrightarrow} \bar{A}_\nu K^{-(\nu+2)}. \tag{11}$$

The two single-variable functions f and ϕ are related through

$$\phi(t) = \int_{-\infty}^\infty f(k)\, e^{ikt}\, \frac{dk}{|k|}, \quad f(k) = \frac{|k|}{2\pi}\int_{-\infty}^\infty \phi(t)\, e^{-ikt} dt. \tag{12}$$

At this moment, we must admit our ignorance about a deeper meaning of the scaling property (9) or (10). But, assuming its validity, we specialize to two typical examples which we designate as

(A) Case of the fast modulation ('motional narrowing' limit),

(B) Case of the slow modulation (Gaussian limit).

A. the fast modulation:

$$\phi(t) = \text{Re}\,(1-it)^{-\frac{\nu}{2}}, \quad f(k) = \frac{1}{2\Gamma(\frac{\nu}{2})}|k|^{\frac{\nu}{2}}\, e^{-|k|}. \tag{13}$$

Note that by means of a Laplace transform and its inversion

$$\begin{aligned}
\int_0^\infty \frac{1}{\Gamma(\frac{\nu}{2})} e^{-k(1+z)} k^{\frac{\nu}{2}-1} dk &= (1+z)^{-\frac{\nu}{2}} \\
\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \frac{e^{zk}}{(1+z)^{\frac{\nu}{2}}} dz &= \begin{cases} \frac{1}{\Gamma(\frac{\nu}{2})} k^{\frac{\nu}{2}-1} e^{-k} & \text{for Re } k > 0 \\ 0 & \text{for Re } k < 0 \end{cases}
\end{aligned}$$

B. the slow modulation:

$$\phi(t) = e^{-\frac{1}{2}t^2}, \quad f(k) = \frac{|k|}{\sqrt{2\pi}}\, e^{-\frac{1}{2}k^2}. \tag{14}$$

It is now clear how these two prototypes lead to the Z–D formulas (1) and (2) by adopting the Wigner type spacing distribution function

$$P_{\text{sp}}(s) = A_\nu s^\nu e^{-s^2/2\sigma_\nu^2}, \tag{15}$$

and by choosing the normalization and scaling constants adequately: It is immediate to obtain the formulas (1) and (2) by inserting (13) and (14), respectively, into the integral transform (3) of the Wigner function (15), where the scaling property (9) plays the decisive role.

3. Generalized (friction-retarded)Langevin Equation

Kubo[6)] discussed a retardation effect on the friction of the Ornstein–Uhlenbeck Brownian motion by writing its Langevin equation as

$$\frac{du}{dt} = -\int_{-\infty}^{\infty} \gamma(t-t')\; u(t')dt' + \frac{1}{m}R(t).$$

The necessity of such a generalization as expressed in the above form stems from the non-white nature of the random force $R(t)$ (i.e. $R(t)$ is not δ–correlated, or its power spectrum nonconstant). Thus it modifies the ordinary fluctuation–dissipation relation between the damping constant and the strength of the white noise such that

$$\int_0^{\infty} \gamma(\tau)\; e^{-i\omega\tau} d\tau = \frac{1}{mkT}\int_0^{\infty} < R(t)R(t+\tau) > e^{-i\omega\tau} d\tau. \tag{16}$$

Kubo called this the *fluctuation–dissipation theorem of the second kind.*

In order to apply this theory to the present problem of describing the variant correlation length, we first write down a set of two–level equation of motion in accordance with the level dynamics[7)] supplemented by a friction term and a random force:

$$\begin{aligned} \frac{dx_i}{dt} &= p_i \qquad i = 1,2 \\ \frac{dp_i}{dt} &= -\frac{\partial V}{\partial x_i} - \int_{-\infty}^{t} \gamma(t-t')\; p_i(t')dt' + R_i(t) \end{aligned} \tag{17}$$

where $V(x_1, x_2) = \dfrac{|L_{12}|^2}{(x_1 - x_2)^2}$ (see [2)]) and $R_i(t)$ $(i = 1,2)$ is assumed to arise from the gradient of the potential $\sum\limits_{n\neq i} V(x_i, x_n)$ $(i = 1,2)$.

Then, let us take the center–of–mass coordinate system:

$$\begin{aligned} X &= \tfrac{1}{2}(x_1 + x_2), & P &= p_1 + p_2 \\ x &= x_2 - x_1, & p &= \tfrac{1}{2}(p_2 - p_1) \end{aligned} \tag{18}$$

This enables us to separate eq. (17) into two sets, and the one for the relative coordinates (x,p) is written as

$$\frac{dx}{dt} = 2p, \quad \frac{dp}{dt} = -\frac{\partial V}{\partial x} - \int_{-\infty}^{t} \gamma(t-t')\; p(t')dt' + r(t) \tag{19}$$

with the fluctuation–dissipation relation (of the 2nd kind) given by

$$\int_0^{\infty} \gamma(\tau)\; e^{-i\omega\tau} d\tau = 2\beta \int_0^{\infty} < r(t)\; r(t+\tau) > e^{-i\omega\tau} d\tau. \tag{20}$$

Here, β denotes the inverse temperature of the equilibrium surrounding the pair of levels which should be defined in the starting level dynamics, and the factor 2 represents the inverse reduced mass (note that each level has a mass unity in our level dynamics). The residual force r in (19), given by $\frac{1}{2}(R_2 - R_1)$, arises certainly because the pair of levels 1 and 2 interact with the other levels, $n \neq 1, 2$, for which the orthogonality $< R_i(t) R_j(t') > = 0$, $i \neq j$, is assumed. Then, the F–D relation (20) recovers its original form

$$\int_0^\infty \gamma(\tau)\, e^{-i\omega\tau} d\tau = \beta \int_0^\infty < R_1(t) R_1(t+\tau) > e^{-i\omega\tau} d\tau.$$

We are now ready to compute the characteristic function of the conditional curvature distribution and hence, with the aid of $P_{\text{sp}}(s)$ in (15), the desired function $P_{\text{curv}}(K)$ with a variant correlation length.

4. Stochastic Modulation Theory for Curvatures

Before going, we argue about what physical meaning should be assigned to the 'time' t in the Langevin equations (17) and (19). In the starting level dynamics, e.g. in Yukawa's formulation[8),7)], one deals with the eigenvalue problem of a Hamiltonian matrix

$$H(\lambda) = H_0 + \lambda H_1 \tag{21}$$

to ask a change of its energy eigenvalues with respect to λ. Here, the parameter λ is dimensionless as far as H_0 and H_1 have the same (energy) dimension. Change the parameter λ to t in the same expression but now H_1 being regarded as a dimensionless quantity:

$$H(t) = H_0 + t H_1.$$

Then, the parameter t now represents an energy variable. Accordingly, in eqs. (17) and (19), the momenta p's are dimensionless and their time derivatives are of the dimension [energy^{-1}]. At the same time, the choice of the dimensionless perturbing matrix H_1 implies that one now has a dimensionless Hamiltonian function for the level dynamics, which is convenient.

It is now possible to identify the curvature K for the pair of levels 1 and 2 with the right–hand side of the Langevin equation (19):

$$\frac{dp}{dt} = \frac{|L|^2}{x^3} - \int_{-\infty}^{t} \gamma(t-t')\, p(t') dt' + r(t) = K(t) \tag{22}$$

This is a fluctuating quantity against energy with its dimension [energy^{-1}]. It is consistent with the starting definition of the curvature (6) apart from the dimensional understanding.

Our task is to calculate the characteristic function $\Phi(t, s)$ of the curvature distribution under the condition specified by (5) such that $\Phi(t, s) = < e^{iKt} | x = s >$. Here, the variable t is the one conjugate to the curvature K in defining the characteristic function i.e. Fourier transform of $P_{\text{curv}}(K, s)$, but now we assert that this variable t is identical to the time variable of the Langevin eq. (19). The reason for this identification can be seen from Kubo's another context of the Brownian motion theory for line shapes, namely the 'random frequency modulation theory'[6)]: He discussed a practical method to compute the

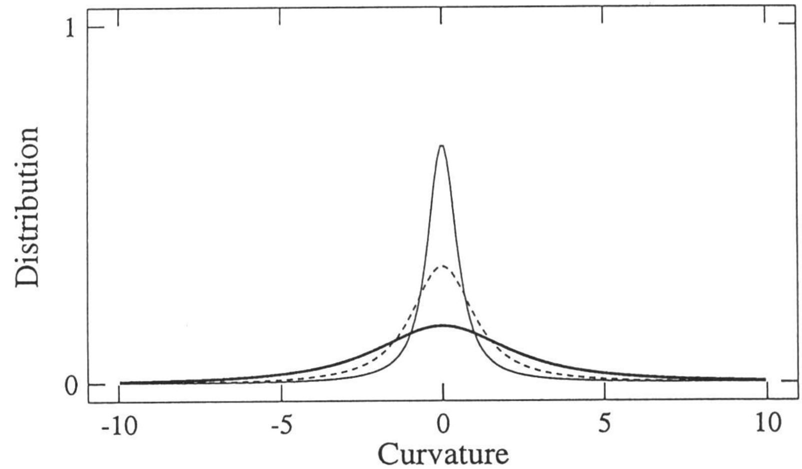


Figure 2: Curvature distribution for GOE statistics obtained from the intermediate characteristic function eq. (26) ($\beta = \pi/2$): $\alpha = 0.5$ (thin line), $\alpha = 1.0$ (dashed line), $\alpha = 2.0$ (thick line).

shape of the frequency spectrum in the mode decomposition of a dynamical variable x into x_ω to satisfy $\frac{d}{dt}x_\omega = i\omega x_\omega$ by proposing to treat this equation as a stochastic equation, or to regard the frequency ω as a stochastic process.

Following Kubo's prescription to replace $e^{i\omega t}$ by $\exp(i\int_0^t \omega(t')dt')$ in the random frequency modulation process, we do make the same treatment of replacing e^{iKt} by $\exp(i\int_0^t K(t')dt')$ which is regarded as a stochastic process, and which is inserted into the definition of the characteristic function $\Phi(t,s) = < e^{iKt}|x(t) = s >$.

Near the equilibrium of the 2-level dynamics ($\rho_e = \frac{1}{Z}e^{-\beta\mathcal{H}}$; $\mathcal{H} = p^2 + \frac{|L|^2}{x^2}$ for the relative coordinate only), we can write as

$$K(t) = \bar{K} + K_{\rm fl}(t), \qquad K_{\rm fl}(t) = r(t) \quad \text{and} \quad \bar{K} = \frac{2|L|^2}{x^3} - \bar{\gamma}p, \tag{23}$$

where

$$< r > = 0 \quad \text{and} \quad \bar{\gamma} = \int_0^\infty \gamma(\tau)d\tau = 2\beta\int_0^\infty < r(t)\, r(t+\tau) > d\tau,$$

implying that the process is stationary. If we further make the assumption that the process $r(t)$ is Gaussian, we can compute $\Phi(t,s)$ as follows:

$$< \exp(i\int_0^t K(t')dt')|x(t) = s> = < e^{i\bar{K}t}|x(t) = s> < \exp(i\int_0^t r(t')dt') >$$

$$= \frac{1}{(1-\frac{2it}{\beta s})^{\frac{\nu}{2}}} \exp\left[-\frac{\bar{\gamma}^2}{4\beta}t^2 - \int_0^t (t-\tau) < r\, r(\tau) > d\tau\right].$$

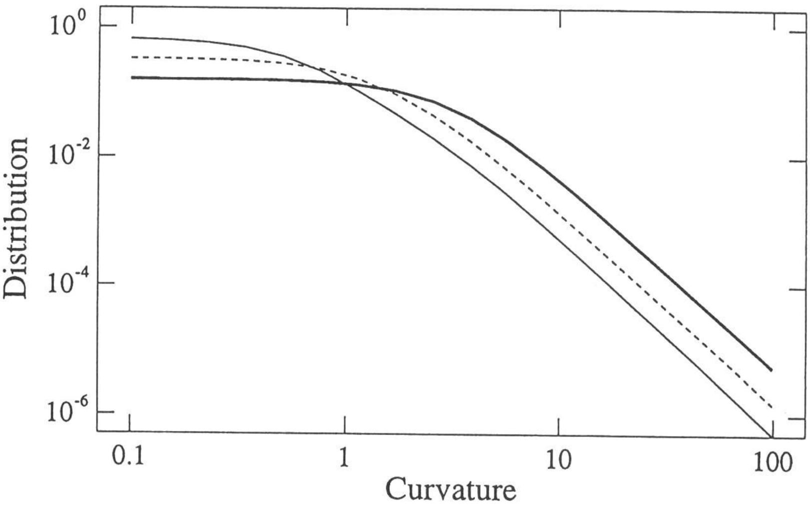


Figure 3: Curvature distribution in a logarithmic scale for GOE statistics obtained from the intermediate characteristic function eq. (26) ($\beta = \pi/2$): $\alpha = 0.5$ (thin line), $\alpha = 1.0$ (dashed line), $\alpha = 2.0$ (thick line). Each straight part corresponds to the K^{-3} line.

We further follow Kubo's ansatz of an exponential decay of the auto-correlation function of $r(t)$ in the exponential, i.e.

$$< r\ r(\tau) > = \frac{1}{2} < R_1 R_1(\tau) > = \frac{\Delta^2}{2} e^{-\tau/\tau_c} \quad \text{hence} \quad \bar{\gamma} = \beta \Delta^2 \tau_c \tag{24}$$

which leads us to an expression

$$\Phi(t,s) = \frac{1}{(1 - \frac{2it}{\beta s})^{\frac{\nu}{2}}} \exp\left[-\frac{\beta \Delta^4}{4} \tau_c^2 t^2 - \frac{\Delta^2}{2} \tau_c \{ t - \tau_c (1 - e^{-t/\tau_c}) \} \right].$$

An inspection of this formula shows that by setting

$$\Delta = \frac{1}{s} \quad \text{and} \quad \Delta \tau_c = \alpha \qquad \text{hence} \quad \tau_c = \alpha s, \tag{25}$$

the function $\Phi(t,s)$ is indeed a single function $\phi(t/s)$ with the two dimensionless parameters β and α:

$$\Phi(t,s) = \phi(\frac{t}{s}) = \frac{1}{(1 - \frac{2it}{\beta s})^{\frac{\nu}{2}}} \exp\left[-\frac{\beta \alpha^2}{4} (\frac{t}{s})^2 - \frac{\alpha}{2} \{ \frac{t}{s} - \alpha (1 - e^{-t/\alpha s}) \} \right]. \tag{26}$$

Here the parameter α represents the relative correlation length in accord with Kubo's parameter to measure the degree of broadening: In the limit $\alpha \to 0$ (motional narrowing limit), $\phi(t)$ reduces to (13) with t replaced by $2t/\beta$, for which the expression (1) results with the scaling constant $B_\nu = \frac{1}{2}\beta\sigma_\nu$. In the opposite situation $\alpha^2 \gg \beta^{-1}$ (Gaussian limit), $\phi(t)$ reduces to (14) with t^2 replaced by $\frac{\beta}{2}\alpha^2 t^2$, for which the expression (2) results with $B'_\nu = \frac{\sigma_\nu}{\alpha}\sqrt{\frac{2}{\beta}}$. Figs. 2, 3 show our numerical studies about the intermediate situation between them.

Thus, our understanding of the nonuniversal feature disclosed in the previous numerical experiments on the parametric motion of levels for different systems is the variant degree of the correlation length of an avoided crossing of the individual pair, which we now believe to be true: The short correlation (rapid modulation) in Case (A) and the long correlation (slow modulation) in Case (B) indeed account for the two pictures illustrated respectively in Fig. 1(a) and 1(b).

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