Statistics of avoided crossings for generic quantum systems

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The distribution of isolated avoided crossings in quantum systems whose classical counterparts possess a mixed phase space of regular and chaotic dynamics is investigated. The distribution function for the width is shown to consist of two components: a near-Gaussian distribution suggested by random matrix theory for the chaotic component and an approximately δ-shaped component originating from tori in the regular portion of phase space. A statistical measure for overlapping avoided crossing based on parametric correlations of energy levels is introduced and shown to be sensitive to the fraction of classically chaotic phase space.

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I. INTRODUCTION

Both experimental [1,2] and numerical [3,4] studies have provided evidence that non-integrability of a classical Hamiltonian system is reflected in the spectra properties of the corresponding quantized systems. On the scale of the average spacing between nearest levels, the distribution of the nearest-neighbor spacing (NNS) has attracted much attention [5]. Berry and Tabor [6] proved rigorously that except for special cases (one-dimensional systems and harmonic oscillators), the NNS distribution for a classically regular system is Poissonian. In the classically chaotic regime, the NNS distribution for a real Hamiltonian system has been shown numerically to follow a Wigner distribution as predicted by the random matrix theory for the Gaussian orthogonal ensemble (GOE) [7].

The local behavior on the finest scale of the quantum spectra, namely, the statistical properties of the avoided crossings (AC) between energy levels, had been proposed in early studies as the fingerprints of classical chaos [8], though at that time only on a qualitative level. Very recently, the width distribution of avoided crossings for the classically completely chaotic system has been investigated quantitatively [9–12] using random matrix theory (RMT), which suggests that the AC distribution is Gaussian for GOE systems. Comparison with numerical experiments showed overall good agreement, however, in the limit of extremely small avoided crossings, deviations from random matrix theory were observed [13].

In the following, we present a study of the AC distribution for "typical" (i.e., generic) Hamiltonian systems whose classical counterparts possess a mixed phase space of regular and chaotic dynamics. We find the integrable component in the classical phase space of a generic system to be reflected in an approximately δ-shaped peak near the origin of the AC width distribution, and find the distribution to change from a δ type to a Gaussian one as the corresponding classical system undergoes a transition from regular to chaotic motion. Furthermore, we introduce a measure for the overlap of nonisolated avoided crossings which is based on the study of correlated motion of energy levels. We show that this measure is sensitive to changes in the underlying classical phase space structure.

II. AVOIDED CROSSINGS AND PARAMETRIC MOTION OF ENERGY LEVELS

Consider a generic system with the symmetry of time reversal described by the Hamiltonian

$$H(\lambda)=H_0+\lambda V\ , \tag{1}$$

where H_0 is a separable Hamiltonian and V is, in general, a nonseparable perturbation. When λ increases, the classical system undergoes a transition from regular to chaotic motion. It is well known [14] that for $H(\lambda)$ with no additional symmetry the quantum levels generally do not cross each other as λ varies. Instead, two levels may approach and recede from each other along two branches of a hyperbola. This behavior is termed avoided crossing. Around the point of the closest approach, λ_c, the distance between two levels can be approximated by the Wigner–von Neumann formula

$$\Delta E=E_{n+1}(\lambda)-E_n(\lambda)=\sqrt{C^2+4\Delta\lambda^2V_0^2}\ , \tag{2}$$

where $C=E_{n+1}(\lambda_c)-E_n(\lambda_c)$ is the minimum distance, $V_0=|V_{n,n+1}(\lambda_c)|$ is the coupling among two levels at the point of the closest approach, and $\Delta\lambda=\lambda-\lambda_c$. Equation (2) corresponds to the "adiabatic" representation of an *isolated* avoided crossing. A more detailed quantitative criterion for an isolated AC will be given below. An alternative diabatic representation follows from the description of the effective 2×2 Hamiltonian for the levels $(n,n+1)$, denoted by (1,2) in the following, by the matrix

$$H_{\rm eff}(\Delta\lambda)=\begin{bmatrix} a\Delta\lambda & \Delta/2 \\ \Delta/2 & -a\Delta\lambda \end{bmatrix}\ , \tag{3}$$

where $\Delta/2$ is the coupling matrix element between two diabatic levels and a is the slope with which the levels approach each other and would cross if Δ would be zero.

Solving the eigenvalue problem (3) and comparing with (2) leads to the correspondence

$$\Delta = C \ , \tag{4a}$$

$$a = V_0 \ . \tag{4b}$$

Note the interchange of the role of (off-) diagonal elements in the (adiabatic) diabatic representation

$$\Delta = 2\langle 1|H_{\text{eff}}|2\rangle_{\text{dia}} = (\langle 2|H|2\rangle - \langle 1|H|1\rangle)_{\text{adia}} \ . \tag{5}$$

Note, furthermore, that Δ and a in (5) are assumed to be independent of $\Delta\lambda$, i.e., the diabatic state vectors $|1,2\rangle$ to be invariant under variation of $\Delta\lambda$ for small $\Delta\lambda$. The latter plays an important role for the correlated motion of energy levels near avoided crossings.

As shown by Pechukas [15], parametric motion of energy levels of (1) as a function of the parameter λ can be described by a set of "equations of motions" in the λ "time,"

$$\frac{d}{d\lambda}E_n = \langle n|V|n\rangle = V_{nn} = p_n \ , \tag{6a}$$

$$\frac{d}{d\lambda}p_n = 2\sum_{i\,(\neq n)} \frac{V_{in}^2}{E_n - E_i} \ , \tag{6b}$$

$$\frac{d}{d\lambda}V_{in} = \sum_{j\,(\neq i,n)} V_{ij}V_{jn}\left[\frac{1}{E_i - E_j} + \frac{1}{E_n - E_j}\right] - \frac{V_{in}(p_i - p_n)}{E_i - E_n} \ . \tag{6c}$$

For systems with time reversal symmetry the coupling matrix elements V_{in} are real and we assume the spectrum to be entirely discrete. It is worth noting that Eq. (6) describes the parametric evolution of the matrix element V_{in} in the adiabatic representation.

We have recently implemented Eq. (6) in numerical studies of the morphology of avoided crossings [16] and of parametric correlations of energy levels [17]. In the following, we use this set of equations for determination of the width distributions and the λ ("temporal") correlation between avoided crossings.

III. WIDTH DISTRIBUTION OF AVOIDED CROSSINGS

For classically completely chaotic, metrically transitive systems, random matrix theory predicts a Gaussian distribution of the width of an avoided crossing. In its simplest form, the underlying argument can be phrased as follows [12]. The two free parameters in H_{eff} in the diabatic representation [Eq. (3)], a and Δ, are independent Gaussian random numbers. Near a quasidegeneracy with $\Delta\lambda \to 0$ (more precisely, $a\Delta\lambda \to 0$,) the width of the avoided crossing is given by Δ [$=C$, Eqs. (2), (4)]. Consequently, RMT predicts

$$P(C) = \frac{2}{\pi\langle C\rangle} e^{-C^2/(\pi\langle C\rangle^2)} \ , \tag{7}$$

with $\langle C\rangle$ the mean value of the width in the ensemble of avoided crossings. In the semiclassical limit, equivalent to the limit $\hbar \to 0$, $\langle C\rangle$ is of the order $\hbar^N$ where N is the number of degrees of freedom of the system [18].

In the quasi-integrable limit, on the other hand, the Hamiltonian system can be quantized via torus [or Einstein-Brillouin-Keller (EBK)] quantization. Invariant tori fill most of the accessible phase space. Energy levels are characterized by complete set of compatible quantum numbers (N actions of the N-torus). Primitive (i.e., nonuniform) semiclassical quantization therefore gives crossings rather than avoided crossings [8]. Uniform quantization lifts these degeneracies and induces small splittings due to dynamical tunneling between tori and narrow phase space zones within which the nonintegrable perturbation destroys tori. The size of avoided crossings in the near-integrable limit is of the order $\exp(-1/\hbar)$ and therefore small compared to the average spacing. On the scale of the average spacing between energy levels, the distribution for these avoided crossings can be approximately described by a δ function

$$P(C) = \delta(C) \ . \tag{8}$$

We note that any other sharply peaked function (on the scale of the mean spacing) is admissible as well, while the advantage of a δ function is that it is without additional free parameters. For generic quantum systems with a mixed classical phase space consisting of regular islands and several chaotic seas, we expect $P(C)$ to consist of two components: One with fraction $1-\gamma$ is formed by avoided crossings involving two adjacent levels from the quantization of the classical tori of regular islands and Eq. (8) applies. The other group with fraction γ involves at least one level embedded in the chaotic sea. The Gaussian distribution [Eq. (7)] should be applicable to this group. Therefore, the distribution for all AC's reads

$$P(C) = (1-\gamma)\delta(C) + \gamma\left[\frac{4D}{\pi}\right]^{1/2} \exp(-DC^2) \ , \tag{9}$$

where D is determined by the average width

$$D = \frac{\gamma^2}{\langle C\rangle^2\pi} \ . \tag{10}$$

This distribution interpolates between a δ distribution [Eq. (8), ($\gamma = 0$)] and a Gaussian distribution [Eq. (7), ($\gamma = 1$)]. The parameter γ can be determined by fitting the results of numerical experiments for quantum spectra. At the same time, we expect γ to be closely related to the fraction of the classically chaotic phase space.

As a model system for testing hypothesis [Eq. (9)] we use the system of two coupled Morse oscillators with [19]

$$\begin{aligned} H_0 &= \sum_{i=1}^{2} H_0^i \ , \\ H_0^i &= P_i^2/2M_i + V_i(r_i) \ , \\ V &= -P_1P_2/m \ , \end{aligned} \tag{11}$$

where M_i are the reduced masses for the two diatomic pairs in the molecule, V_i are the corresponding Morse potentials, and m is the mass of the central atom. This system provides a simple model for the vibronic motion of

linear triatomic molecules and has been extensively studied as a model for the quantum mechanics of a classically chaotic system with two degrees of freedom [20]. We used the molecular parameters for H—C—C which provide 770 bound states in the integrable limit. The coupling to the continuum is neglected. More detailed information on our numerical calculation is given in Ref. [21]. It is important that the interval of λ within which the avoided crossings are counted must be small compared to the range of λ when the classical phase space of Eq. (1) undergoes structural changes.

The study of the parametric evolution of the spectrum [Eq. (6)] is particularly convenient to identify isolated avoided crossings. Only those avoided crossings should be included which are dominated by a two-level interaction such that two-level approximation [Eq. (2)] is locally valid near the point of the closest approach λ_c. The validity of the two-level approximation can be easily tested for each avoided crossing within our calculation by requiring that the residual forces exerted by other levels [see Eq. (6b)] on the two levels in question, F_N, are negligible compared to the dominant two-level force F_2 between the two levels, i.e.,

$$F_N=\max_{s=n,n+1}\left\{\left|2\sum_{k\ (\neq n,n+1)}\frac{V_{k,s}^2}{E_s-E_k}\right|\right\}$$
$$\ll F_2=\frac{2V_{n,n+1}^2}{E_{n+1}-E_n} \tag{12}$$

for $\lambda\approx\lambda_c$. We have fund that for $F_N/F_2<0.1$ the two-level approximation is accurate enough and therefore used this criterion to choose avoided crossings. We note that the results are stable against the variation of the cutoff criterion, provided that $F_N\ll F_2$.

Figure 1(a) displays the AC distribution in the perturbative regime ($0\le\lambda\le0.1$) where C is in units of the average spacing. The circles are the values of Eq. (9) averaged over each window of size $\Delta C=0.05$ and the numerical results of the system for coupled Morse oscillators are represented by histograms. The dominant feature is clearly the sharp peak near the origin $C=0$. Note the peak width is not intrinsic but is determined by the window size ΔC. The sharp peak near the origin signifies the approximate separability and the persistence of Kol'mogorov-Arnol'd-Moser (KAM) tori in the classical phase space. A very weak Gaussian component at large C is recognizable. For strong perturbations ($0.5\le\lambda\le0.8$) chaotic motion becomes prevalent, though some regular islands still exist (see Fig. 2). Figure 1(b) shows that the corresponding AC distribution consists of two components: a dominant Gaussian tail and a small peak near the origin, as predicted by distribution Eq. (9). Figure 2 displays the λ dependences of quantum parameter γ and the fraction of classical chaotic phase space [21] $Q_{\rm cl}$ in the energy hypershells within which the quantum energy levels lie. We averaged the fraction $Q_{\rm cl}$ within each window of $\delta\lambda=0.1$. One can see that γ closely follows $Q_{\rm cl}$. The AC distribution changes from a δ type to a Gaussian one as the corresponding classical system undergoes a transition from regular to chaotic motion.

The validity of the RMT prediction [Eq. (7)] for small C cannot be tested, however, for a mixed system since the region near the origin is always "overshadowed" by the δ contribution due to regular islands. Only in the limit of completely chaotic systems, or systems whose regular islands are too small to accommodate quantum states, does the $C\to0$ limit of RMT become accessible. For several such systems (strongly "kicked" top, billiards, hydrogen in strong magnetic field [22]) recent investigations [12,13] found systematic deviations which were detected in the cumulative distribution

$$I(C)=\int_0^C dC'P(C')\ . \tag{13}$$

The width of the avoided crossings for billiards has been recently linked to very long periodic orbits [23]. According to the GOE result [Eq. (7), or Eq. (9) with $\gamma=1$], $I(C)$ should be proportional to C in the limit of small C for chaotic systems. Using a sample of $\approx10\,000$ AC's, it was shown in Ref. [12] that $I(C)$ does not grow linearly with C. As found by Goldberg and Schweizer [13], $I(C)$ grows instead quadratically with C for small C, i.e.,

$$P(C)=\frac{d}{dC}I(C)\propto C\ ,\quad C\to0\ . \tag{14}$$

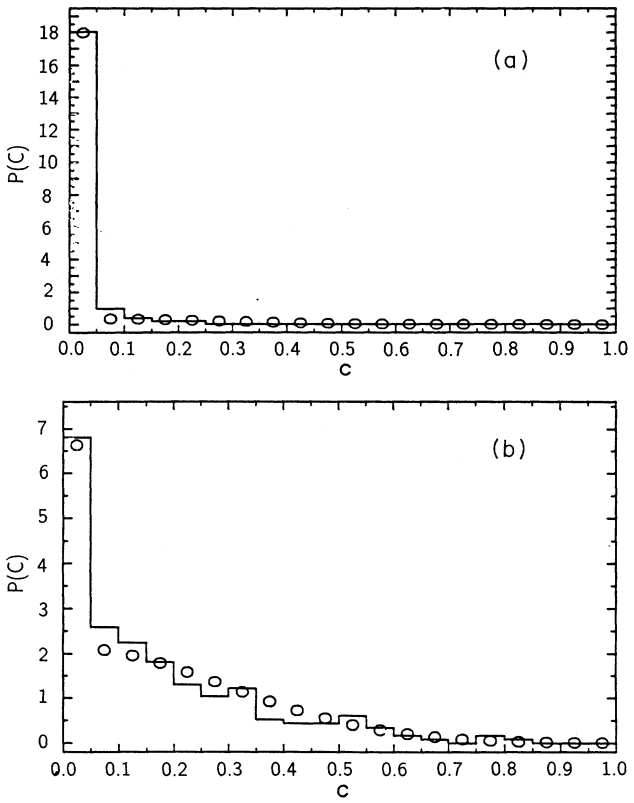

FIG. 1. The AC distribution (a) in the near-integrable regime ($0\le\lambda\le0.1$) and (b) in mostly chaotic regime ($0.5\le\lambda\le0.8$) where C is in units of the average level spacing. The circles are the averages of the distribution function Eq. (9) over the window of the histogram (0.05 of mean spacing). The numerical results for coupled Morse oscillators are given by histograms.

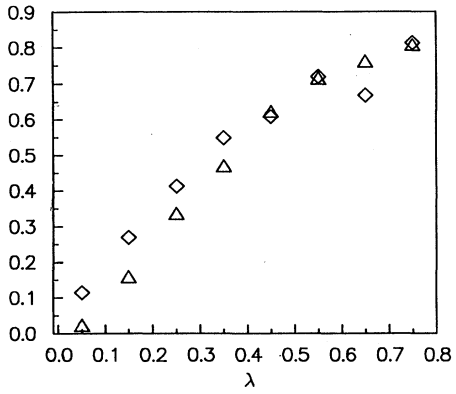

FIG. 2. Quantum parameter γ (diamond) and the fraction of classically chaotic phase space in the energy shells contributing to the energy level statistics, $Q_{\rm cl}$, (triangles) as a function of λ for coupled Morse oscillators.

The origin of this deviation is not yet clear. The proposal that they are due to insufficient ensemble size can be clearly rule out [24]. As recently suggested, another possibility would be numerical errors in the determination of the width distribution [25]. The third possibility is strong parametric correlations among matrix elements and effects of overlapping avoided crossings [24]. We will in the following analyze the distribution of nonisolated avoided crossings.

IV. OVERLAPPING AVOIDED CROSSINGS

A multitude of overlapping avoided crossings has been proposed from early on as a signature of classical chaos in quantum spectra [8]. Numerical calculations supported this criterion qualitatively, but a quantitative description for the amount of overlap has only recently begun to develop. One measure is the mixing angle describing the incomplete exchange of diabatic state vectors across an avoided crossing due to the presence of other nearby levels [26]. In the following we introduce a measure that is solely based on the parametric variation of the energy levels without explicit reference to wave functions.

The parametric equations of motion [Eq. (6)] provide a convenient framework to analyze the parametric correlations among matrix elements. Specializing to the two-level system involved in an isolated avoided crossing Eq. (6) becomes

$$\Delta\dot{E}=p \ , \tag{15a}$$

$$\Delta\ddot{E}=4\frac{V_{12}^2}{\Delta E} \ , \tag{15b}$$

$$\dot{V}_{12}=-V_{12}\frac{p}{\Delta E} \ . \tag{15c}$$

The Wigner–von Neumann formula for $\Delta E(\lambda)$ [Eq. (2)] solves the system (15). Moreover, we find an explicit expression for the $\Delta\lambda$-dependent adiabatic coupling matrix element

$$V_{12}(\Delta\lambda)=V_0\frac{C}{\sqrt{C^2+4(\Delta\lambda V_0)^2}} \ . \tag{16}$$

From (15c) follows that $\Delta E(\Delta\lambda)V_{12}(\Delta\lambda)$ is a constant of λ motion, in particular

$$\Delta E(\Delta\lambda)V_{12}(\Delta\lambda)=V_0C \tag{17}$$

for all $\Delta\lambda$. In the limit of "large" $\Delta\lambda$ (but still within the range of validity of the two-level approximation), i.e.,

$$|\Delta\lambda|\gg\frac{C}{2|V_0|} \ , \tag{18}$$

the matrix elements become

$$V_{12}(\Delta\lambda)\simeq\frac{C}{2\Delta\lambda}\mathrm{sgn}(V_0\Delta\lambda) \ , \tag{19a}$$

$$\Delta E(\Delta\lambda)\simeq 2|\Delta\lambda V_0| \ . \tag{19b}$$

Equations (18) and (19) are used to define a measure for overlapping avoided crossings. The latter are characterized by a breakdown of the Wigner–von Neumann formula for isolated avoided crossings [Eq. (2)]. The two-level approximation [Eq. (15)] underlying Eq. (2) becomes invalid due to the presence of levels with which one of the two levels undergoes a subsequent avoided crossing. The avoided crossing can be considered to be isolated if the asymptotic form of the level separation [Eq. (19)] is reached prior to the encounter with other levels. Denoting the distance between two adjacent avoided crossings in λ parameter space of the same level by $\Delta\lambda_0$, the ratio

$$R=\left|\frac{C}{2\Delta\lambda_0 V_0}\right| \tag{20}$$

measures the amount of overlap. An isolated avoided crossing corresponds to $R\ll 1$ while $R\simeq 1$ implies strong overlap.

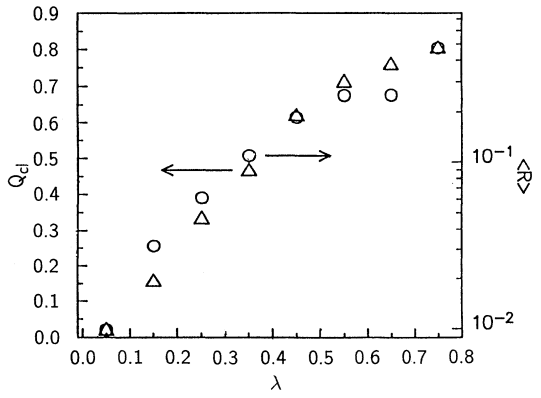

FIG. 3. Overlap parameter $\langle R\rangle$ (circle) and the fraction of classically chaotic phase space in the energy shells contributing to the energy level statistics, $Q_{\rm cl}$, (triangles) as a function of λ for coupled Morse oscillators.

The ensemble average R provides a measure of the overlap of the avoided crossings for the system. Because R varies by orders of magnitude in classical transition regime, it is convenient to employ for an ensemble of avoided crossings the geometrical mean

$$\langle R \rangle = (R_1 R_2 \cdots R_N)^{1/N} . \tag{21}$$

Figure 3 depicts $\langle R \rangle$ as a function of λ averaged over all AC's within a given window of $\delta\lambda = 0.1$. In the perturbative regime ($0 \leq \lambda \leq 0.1$), $\langle R \rangle \approx 10^{-2}$ indicating the avoided crossings are mainly isolated. When $0.7 \leq \lambda \leq 0.8$, $\langle R \rangle$ has risen to $\simeq 0.5$ indicating the prevalence of overlapping avoided crossings. In order to illustrate the correspondence to the classical phase space structure we have overlaid the fraction of classical chaotic phase space $Q_{\rm cl}$. The relative position and scale between the two axes (left-hand side $Q_{\rm cl}$ and right-hand side $\langle R \rangle$) were determined by a least-χ^2 fit

$$\min_{(A,B)} \sum_i \{\log_{10}\langle R \rangle(\lambda_i) - [A Q_{\rm cl}(\lambda_i) + B]\}^2 .$$

As expected, the amount of overlap is directly correlated with the fraction of chaotic phase space.

V. CONCLUSIONS

The distribution function for the width of avoided crossings, $P(C)$, for a Hamiltonian with mixed phase space is shown to consist of an approximately δ-shaped component associated with the regular fraction of phase space and an approximately Gaussian distribution for the chaotic fraction of phase space. A measure for overlap of avoided crossings is introduced and shown to be closely correlated with the fraction of chaotic phase space.

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