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Statistics of multiple avoided crossings

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Abstract. We consider the energy levels of a generic quantum mechanical system with Hamiltonian $\hat{H}$ depending on a parameter X. If the energy levels E_n are plotted as a function of X, the curves do not cross. The points of closest approach are called avoided crossings; these have a distinctive geometry and are important because they determine the limits of applicability of the adiabatic theorem. This paper describes some theoretical results on the parameter space density of avoided crossings, for systems with the spectral statistics of the Gaussian orthogonal ensemble (GOE). These results are in good agreement with numerical experiments.

1. Introduction

Figure 1 is a graph of the energy levels of a generic quantum mechanical system (to be described later), plotted as a function of a parameter X which enters into the

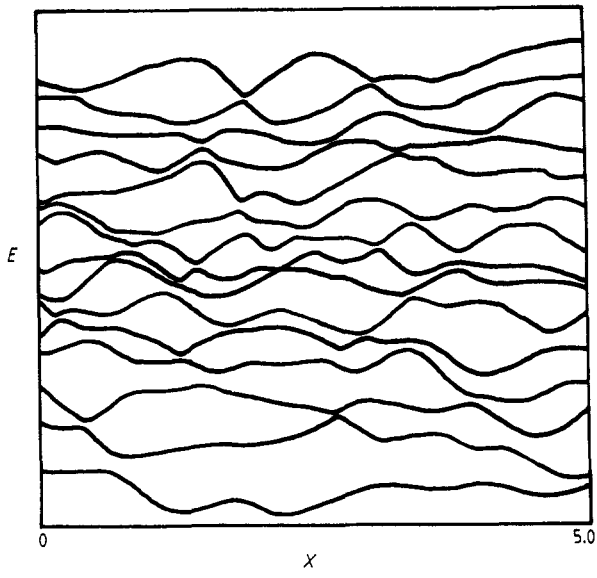

Figure 1. Illustrating the dependence of the energy levels E of a typical quantum mechanical system on a parameter X. The curves never intersect each other, but they do approach each other at events called avoided crossings (in this picture there is one apparent crossing, but this is an artefact due to the finite width of the lines). The system is the GOE random matrix model described in § 2: the dimension of the matrix is $N = 15$ and the variance parameters are $\mu = \sigma = 1$.

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Hamiltonian. The graph has two distinctive features: the curves intersect with probability zero, but they do approach each other as if they were going to cross, as shown in figure 2. This paper will describe some universal statistical properties of multiple avoided crossings, such as those shown in figure 1: the density of avoided crossings will be calculated as a function of the gap size and asymptotic slopes, and the theoretical results are shown to be in good agreement with numerical experiments. The avoided crossings are of physical importance because they determine the limit of applicability of the adiabatic theorem (Bohm 1951). This theorem states that, if the parameter X is varied sufficiently slowly, the modulus of the amplitude $\langle n(X)|\psi\rangle$ remains almost constant, where $|n(X)\rangle$ is the nth eigenstate of the instantaneous Hamiltonian, $H(X(t))$. The condition for the adiabatic theorem to be valid is that for each pair of energy levels

$$(E_{n+1}-E_n)^2 \gg \left(\frac{\partial \hat{H}}{\partial X}\right)_{n,n+1} \hbar \dot{X} \tag{1.1}$$

for all X, where $\dot{X}$ is the rate of change of X. The adiabatic theorem breaks down at narrowly avoided crossings, where the $E_{n+1}-E_n$ is small (Zener 1932). The density of avoided crossings determines how frequently this breakdown is expected to occur (Wilkinson 1988).

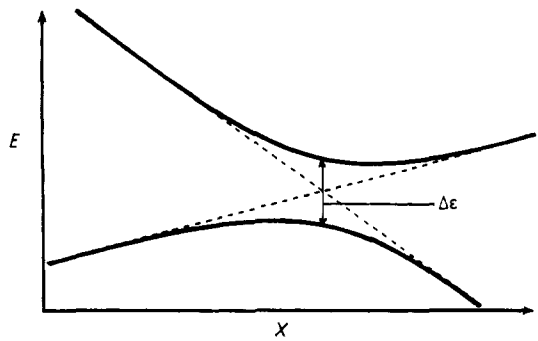

Figure 2. An isolated avoided crossing. The avoided crossing is characterised by three parameters: $\Delta\varepsilon$ is the size of the gap and A, B are, respectively, the difference and mean of the two asymptotic slopes (broken lines).

It is by now well established that ensembles of random matrices can be used to model the statistical properties of energy levels of generic or typical quantum systems, i.e. systems without any symmetries or constants of motion which enable quantum numbers other than the level number to be assigned. The theory of these random matrix ensembles and their successful application to nuclear spectroscopy are described in a reprint volume edited by Porter (1965). These theories have also been applied successfully to systems with a chaotic classical limit (Bohigas *et al* 1984). Although the full range of systems for which random matrix theories are valid has not yet been established, they certainly form an important universality class. Both the theoretical and the numerical work described in this paper use the Gaussian orthogonal ensemble (GOE) as a model for a generic system with time-reversal symmetry. A parameter-dependent version of the GOE model is described in § 2.

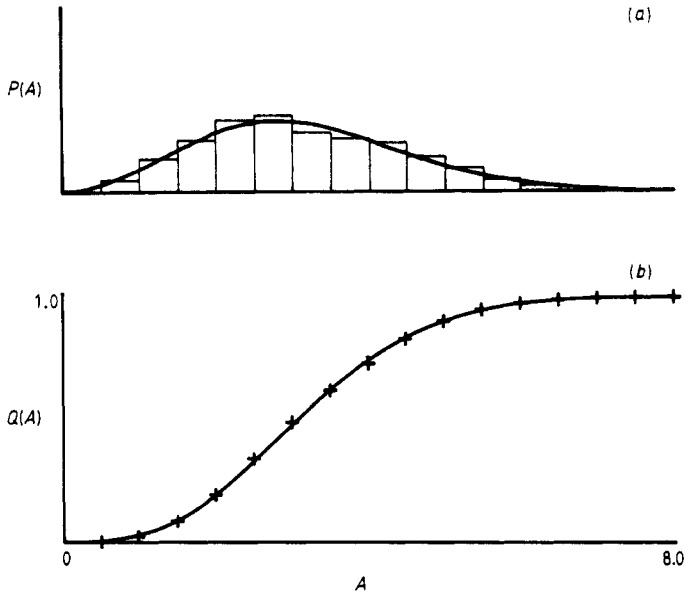

Figure 3. The empirical probability distribution (a) and cumulant distribution (b) of the asymptotic difference in slopes of energy levels undergoing an avoided crossing, compared with the theoretical predictions (full curves). Only avoided crossings for which $n_0\Delta\varepsilon < 0.3$ were included. The sample size was 1557 and the width of the bins is 0.5.

If the system has symmetries, or constants of motion in addition to the Hamiltonian, the energy levels do cross as a parameter is varied: this is caused by the vanishing of some of the off-diagonal matrix elements of $\partial H/\partial X$. These systems are not considered further in this paper.

An isolated avoided crossing is parametrised by three variables: the size of the gap at the closest approach of the energy levels, and two variables describing the asymptotic slope of the curves (see figure 2). In the case of a system of multiple avoided crossings, these asymptotic slopes can still be defined for avoided crossings with a very small gap, because the geometry is locally like that illustrated in figure 2. Section 3 will describe a theory for the density of avoided crossings as a function of these three parameters. The theory is restricted to small values of the gap parameter $\Delta\varepsilon$, because for large $\Delta\varepsilon$ the slope parameters are not well defined.

The results of numerical experiments are compared with the theoretical predictions in § 4.

2. A parameter-dependent random matrix model

The model is based on the Gaussian orthogonal ensemble (GOE), which is an ensemble of real symmetric $N \times N$ matrices $\tilde{H}$ with the following properties:

(i) the matrix elements H_{ij} are independently Gaussian distributed;

(ii) the probability density of the ensemble is invariant under orthogonal transformations, $\tilde{H} \to \tilde{H}' = \tilde{O}^{-1}\tilde{H}\tilde{O}$, where $\tilde{O}$ is an orthogonal matrix.

Porter (1965) argues that this ensemble is appropriate for describing the spectral statistics of typical systems with time-reversal symmetry, and shows that it is uniquely

realised by choosing the variances and means of the H_{ij} as follows:

$$\langle (H_{ij} - \langle H_{ij} \rangle)^2 \rangle = \mu^2 (1 + \delta_{ij}) \tag{2.1}$$

$$\langle H_{ij} \rangle = \text{constant} \times \delta_{ij} \tag{2.2}$$

where $\langle\ \rangle$ denotes an ensemble average, δ_{ij} is the Kronecker delta and μ is a constant. Without loss of generality, we can take the constant in (2.2) to be zero, so that the distribution of eigenvalues is symmetric about $E = 0$. The density of states is given by

$$n(E) = \left\langle \sum_{n=1}^{N} \delta(E - E_n) \right\rangle = \frac{\sqrt{N}}{\pi\mu} \left(1 - \frac{E^2}{4\mu^2 N} \right)^{1/2} \tag{2.3}$$

in the limit $N \to \infty$. This result is called Wigner's semicircle law (Porter 1965).

Our aim is to modify the GOE described above so that the matrix elements depend smoothly on a parameter X. To achieve this we obtain the matrix elements by smoothing a white noise signal with an appropriate filter function:

$$H_{ij}(X) = \mu\beta_{ij} \int_{-\infty}^{\infty} \mathrm{d}X' f(X - X') W_{ij}(X') \tag{2.4}$$

where $\beta_{ij} = 1 + (\sqrt{2} - 1)\delta_{ij}$, and the W_{ij} are uncorrelated white noise with unit intensity:

$$\langle W_{ij}(X) W_{i'j'}(X') \rangle = \delta_{ii'}\delta_{jj'}\delta(X - X'). \tag{2.5}$$

It is convenient to use a 'causal' filter function $f(X)$, i.e. one which is zero for $X < 0$, since this facilitates the numerical simulation of (2.4).

The existence of derivatives of the matrix elements with respect to X is related to the smoothness of the filter function $f(X)$: if $f(X)$ has a discontinuity in its nth derivative, then $\mathrm{d}^n H_{ij}/\mathrm{d}X^n$ exists but is not continuous. For the calculations described here it was sufficient for the second derivative of the H_{ij} to exist, so that $f(X)$ should have a continuous first derivative. The simplest causal function satisfying this requirement is

$$f(X) = \begin{cases} aX^2 \mathrm{e}^{-bX} & X \geqslant 0 \\ 0 & X < 0. \end{cases} \tag{2.6}$$

The constants a, b are chosen such that the variance of the H_{ij} is given by (2.1), and the variance of the derivative is given by

$$\left\langle \left(\frac{\mathrm{d}H_{ij}}{\mathrm{d}X} \right)^2 \right\rangle = (1 + \delta_{ij})\sigma^2 \tag{2.7}$$

where σ is a constant. The values of the constants a, b which satisfy these conditions are evaluated in the appendix.

The theoretical results described in § 3 assume that we know the statistical distribution of the matrix elements

$$\left(\frac{\partial H}{\partial X} \right)_{nm} = \left\langle n \left| \frac{\partial \hat{H}}{\partial X} \right| m \right\rangle \tag{2.8}$$

where $|n\rangle$, $|m\rangle$ are eigenvectors of the Hamiltonian H. In the context of our random matrix model, these matrix elements are

$$\left(\frac{\mathrm{d}\tilde{H}'}{\mathrm{d}X} \right)_{nm} = \sum_{i,j=1}^{N} \psi_i^n \left(\frac{\mathrm{d}\tilde{H}}{\mathrm{d}X} \right)_{ij} \psi_j^m \tag{2.9}$$

where ψ_i^n is the ith component of the nth eigenvector of the matrix $\tilde{H}$. From (2.7), we see that the derivative matrix $\mathrm{d}\tilde{H}'/\mathrm{d}X$ is representative of a GOE with variance parameter σ^2, and from (2.9) we see that $(\mathrm{d}\tilde{H}'/\mathrm{d}X)_{nm}$ is an orthogonal transformation of $(\mathrm{d}H/\mathrm{d}X)_{ij}$. It follows from the definition of the GOE that the matrix $(\mathrm{d}\tilde{H}'/\mathrm{d}X)_{nm}$ is also representative of a GOE. The matrix elements $(\mathrm{d}\tilde{H}/\mathrm{d}X)_{nm}$ are therefore independently Gaussian distributed, with variance

$$\left\langle \left(\frac{\mathrm{d}H'}{\mathrm{d}X} \right)_{nm}^2 \right\rangle = (1+\delta_{ij})\sigma^2. \tag{2.10}$$

3. Theory of density of avoided crossings

In the neighbourhood of an isolated avoided crossing, the dependence of the energy levels $E^{\pm}$ on the parameter X has the form of a hyperbola

$$E^{\pm}(X) = E_0 + B(X - X_0) \pm \tfrac{1}{2}[\Delta\varepsilon^2 + A^2(X - X_0)^2]^{1/2}. \tag{3.1}$$

A derivation will be given shortly. The parameters can be interpreted as follows: $\Delta\varepsilon$ is the size of the energy gap, B and A are, respectively, the mean and difference of the asymptotic slopes of the two curves, and E_0 and X_0 describe the position of the avoided crossing. Our aim will be to derive an expression for the density of avoided crossings expressed as a function of the three parameters $\Delta\varepsilon$, A, B. This density, $N(A, B, \Delta\varepsilon)$, is defined as follows: the number of avoided crossings per unit parameter X, per energy level, with $A, B, \Delta\varepsilon$ in the intervals $[A, A+\mathrm{d}A]$, $[B, B+\mathrm{d}B]$, $[\Delta\varepsilon, \Delta\varepsilon+\mathrm{d}\Delta\varepsilon]$, is $N(A, B, \Delta\varepsilon)\,\mathrm{d}A\,\mathrm{d}B\,\mathrm{d}\Delta\varepsilon$.

The density of avoided crossings can be calculated by the following method. We assume that the energy levels E_n and the matrix elements of the operator $\partial H/\partial X$ have been evaluated at $X = 0$. Using these values, we can calculate the parameters of avoided crossings with X_0 close to zero: this is done by applying degenerate perturbation theory to pairs of energy levels which are very close together. The density of avoided crossings is then given by the probability that a pair of levels exhibit an avoided crossing with X_0 between 0 and ΔX, divided by the size of the interval ΔX. If A', B', $\Delta\varepsilon'$ are the actual values of A, B, $\Delta\varepsilon$ for a given avoided crossing, then

$$\begin{aligned} &N(A, B, \Delta\varepsilon)\,\mathrm{d}A\,\mathrm{d}B\,\mathrm{d}\Delta\varepsilon \\ &\quad = \lim_{\Delta X \to 0} P[0 < X_0 < \Delta X,\ A < A' < A + \mathrm{d}A, \\ &\qquad \times B < B' < B + \mathrm{d}B,\ \Delta\varepsilon < \Delta\varepsilon' < \Delta\varepsilon + \mathrm{d}\Delta\varepsilon] \end{aligned} \tag{3.2}$$

where $P[\ ]$ denotes a probability.

In order to calculate the probability appearing on the RHS of (3.2) it is necessary to know how the parameters of the avoided crossing, X_0, A', B', $\Delta\varepsilon'$, are related to the eigenvalues E_n and the matrix elements $(\partial H/\partial X)_{nm}$, and also the probability distribution of these latter quantities.

Consider first the relationship between the parameters of the avoided crossing and the energy levels and matrix elements. Assume that the eigenvalues E_n and E_{n+1} are very nearly equal at $X = 0$. In the neighbourhood of this point, the two energy levels

can be described by degenerate perturbation theory: the energy levels are eigenvalues of the 2×2 matrix

$$\hat{H}=\begin{bmatrix} e^{+} & h \\ h & e^{-} \end{bmatrix}. \tag{3.3}$$

It is sufficient to use a linear approximation to model the X dependence of the matrix elements:

$$e^{-}=e_0^{-}+e_1^{-}X=E_n+\left(\frac{\partial \hat{H}}{\partial X}\right)_{nn}X \tag{3.4}$$

$$e^{+}=e_0^{+}+e_1^{+}X=E_{n+1}+\left(\frac{\partial \hat{H}}{\partial X}\right)_{n+1,n+1}X \tag{3.5}$$

$$h=h_1X=\left(\frac{\partial \hat{H}}{\partial X}\right)_{n,n+1}X. \tag{3.6}$$

The energy levels and matrix elements on the RHS are evaluated at $X=0$, so that $h(0)=0$. The eigenvalues of (3.3) are given by

$$E^{\pm}(X)=\tfrac{1}{2}(e^{+}+e^{-})\pm\tfrac{1}{2}(e^2+4h^2)^{1/2} \tag{3.7}$$

where

$$e=e^{+}-e^{-}=e_0+e_1X. \tag{3.8}$$

Equation (3.7) is of the same form as our standard parametrisation of the avoided crossing, (3.1). Substituting (3.4)-(3.6) into (3.7), and comparing the resulting expression with (3.1), we find the following equations relating the parameters of the avoided crossing to the energy levels and matrix elements at $X=0$:

$$A=(e_1^2+4h_1^2)^{1/2} \tag{3.9}$$

$$X_0=e_0e_1/A^2=e_0e_1/(e_1^2+4h_1^2) \tag{3.10}$$

$$\Delta\varepsilon=(e_0^2-A^2X_0^2)^{1/2}=2h_1e_0/(e_1^2+4h_1^2)^{1/2} \tag{3.11}$$

$$B=\tfrac{1}{2}(e_1^{+}+e_1^{-}). \tag{3.12}$$

Next, consider the probability distribution of the quantities e_0, e_1, h_1 appearing in the RHS of these four equations. We expect the matrix elements of $\partial H/\partial X$ to be representative of the GOE (see discussion at the end of § 2). The quantities e_1^{+}, e_1^{-} and h_1 are therefore independently Gaussian distributed with variances $2\sigma^2$ and σ^2, respectively (cf (2.1) and (2.2)). The mean values of e_1^{+} and e_1^{-} are identical (and have been set equal to zero in our random matrix model). It follows that h, $e_1=e_1^{+}-e_1^{-}$ and $B=\tfrac{1}{2}(e_1^{+}+e_1^{-})$ are independently Gaussian distributed, with variances σ^2, $4\sigma^2$ and $2\sigma^2$, respectively. The mean values of h_1 and e_1 are zero, but the mean of B need not be zero, although it is zero in our random matrix model. The joint probability density of these quantities is therefore

$$P[e_1,h_1,B]\,\mathrm{d}e_1\,\mathrm{d}h_1\,\mathrm{d}B$$
$$=(2\pi)^{-3/2}2^{-3/2}\sigma^{-3}\exp[-(e_1^2+4h_1^2+2B^2)/8\sigma^2]\,\mathrm{d}e_1\,\mathrm{d}h_1\,\mathrm{d}B. \tag{3.13}$$

The other quantity appearing on the RHS of (3.9)-(3.12) is e_0, the separation of the two eigenvalues at $X=0$. The probability density for this quantity is called the level

spacing distribution, and has been intensively studied in random matrix theory. For GOE matrices, the form of $P[e_0]$ is known exactly for small e_0 (satisfying $n_0 e_0 \ll 1$, where n_0 is the smoothed density of states)

$$P[e_0]\,de_0 = \tfrac{1}{6}\pi^2 n_0^2 e_0\,de_0 \tag{3.14}$$

(Dyson 1962). The level spacing, e_0, is independent of the other variables, e_1, h_1, B, because they are related to two independent random matrices, H and $\partial H/\partial X$, respectively. The overall probability density for the variables appearing on the RHS of equations (3.9)-(3.12) is therefore the product of (3.13) and (3.14).

We can now write down an explicit expression corresponding to (3.2):

$$\begin{aligned} &N(A, B, \Delta\varepsilon)\,dA\,dB\,d\Delta\varepsilon \\ &\quad = \lim_{\Delta X \to 0} \frac{1}{\Delta X} \int_{-\infty}^{\infty} de_1 \int_{-\infty}^{\infty} dh_1 \int_{-\infty}^{\infty} dB\, P[e_1, h_1, B] \int_0^{\infty} de_0\, P[e_0] \\ &\quad\quad \times \delta(A - A')\delta(\Delta\varepsilon - \Delta\varepsilon')\theta(X_0')\theta(\Delta X - X_0') \end{aligned} \tag{3.15}$$

where A', $\Delta\varepsilon'$ and X_0' are functions of e_0, e_1, h_1 given by (3.9)-(3.11), respectively, and $\theta(X)$ is the unit increasing step function. In the limit $\Delta X \to 0$, the 'top hat function' in (3.15) obtained by taking the product of two θ functions can be replaced by a Dirac delta function, and the probability density of B can be factored out of the integral immediately:

$$\begin{aligned} &N(A, B, \Delta\varepsilon)\,dA\,dB\,d\Delta\varepsilon \\ &\quad = P[B]\,dB \int_{-\infty}^{\infty} de_1 \int_{-\infty}^{\infty} dh_1\, P[e_1, h_1] \int_0^{\infty} de_0 \\ &\quad\quad \times P[e_0]\delta(A - A')\delta(\Delta\varepsilon - \Delta\varepsilon')\delta(X_0')\,dA\,d\Delta\varepsilon \end{aligned} \tag{3.16}$$

where

$$P[B]\,dB = (2\pi)^{-1/2} 2^{-1/2} \sigma^{-1} \exp(-B^2/4\sigma^2)\,dB. \tag{3.17}$$

The evaluation of the triple integral in (3.16) is facilitated by making a change of variables $(e_1, h_1) \to (r, \theta)$:

$$e_1 = r\cos\theta \qquad h_1 = \tfrac{1}{2} r \sin\theta. \tag{3.18}$$

Using these new variables, and substituting the probability densities from (3.13) and (3.14), we obtain

$$\begin{aligned} &N(A, B, \Delta\varepsilon)\,dA\,dB\,d\Delta\varepsilon \\ &\quad = P[B]\,dB \frac{\pi n_0^2}{24\sigma^2} \int_0^{\infty} de_0\, e_0 \int_0^{2\pi} d\theta \int_0^{\infty} dr\, r \\ &\quad\quad \times \exp(-r^2/8\sigma^2)\delta(r - A)\delta(e_0 \sin\theta - \Delta\varepsilon)\delta(e_0 \cos\theta/r)\,dA\,d\Delta\varepsilon. \end{aligned} \tag{3.19}$$

Using the result

$$\delta(e_0 \cos\theta/r) = (r/e_0)\delta((\theta - \pi/2) \bmod \pi) \tag{3.20}$$

we can evaluate to integrals over (r, θ), then the integral over e_0

$$\begin{aligned} &N(A, B, \Delta\varepsilon)\,dA\,dB\,d\Delta\varepsilon \\ &\quad = P[B]\,dB \frac{\pi n_0^2}{24\sigma^2} \int_0^{\infty} de_0\, e_0 A\delta(e_0 - \Delta\varepsilon)\frac{A}{e_0} \exp(-A^2/8\sigma^2)\,dA\,d\Delta\varepsilon \\ &\quad = P[B]\,dB \frac{\pi n_0^2}{24\sigma^2} A^2 \exp(-A^2/8\sigma^2)\,dA\,d\Delta\varepsilon \end{aligned} \tag{3.21}$$

where $P[B]$ is given by (3.17). This expression is only valid for small $\Delta\varepsilon$ satisfying $\Delta\varepsilon n_0 \ll 1$.

4. Numerical experiments

It would require an immense amount of data to verify (3.21), the expression for the joint density function $N(A, B, \varepsilon)$, since this depends on three variables. Instead, numerical experiments were carried out to test two partial statistics derived from (3.21). The first of these partial statistics was the density of avoided crossings with gap sizes between 0 and $\Delta\varepsilon$, irrespective of the values of A and B. This partial density is given by

$$F(\Delta\varepsilon) = \int_0^{\Delta\varepsilon} \mathrm{d}\Delta\varepsilon' \int_0^{\infty} \mathrm{d}A \int_{-\infty}^{\infty} \mathrm{d}B\, N(A, B, \Delta\varepsilon')$$
$$= \tfrac{1}{3}\pi(\tfrac{1}{2}\pi)^{1/2}\sigma n_0^2 \Delta\varepsilon. \tag{4.1}$$

Evaluating $F(\Delta\varepsilon)$ checks that $N(A, B, \Delta\varepsilon)$ is independent of $\Delta\varepsilon$ and verifies that the prefactor is correct. The second partial statistic was the probability distribution of A at avoided crossings with gap sizes less than $\Delta\varepsilon$:

$$P[A]\,\mathrm{d}A = \frac{1}{F(\Delta\varepsilon)} \int_0^{\Delta\varepsilon} \mathrm{d}\Delta\varepsilon' \int_{-\infty}^{\infty} \mathrm{d}B\, N(A, B, \Delta\varepsilon)\,\mathrm{d}A$$
$$= \frac{1}{4\sqrt{2\pi}\sigma^3} A^2 \exp(-A^2/8\sigma^2)\,\mathrm{d}A \tag{4.2}$$

for small $\Delta\varepsilon$. This statistic was examined because the dependence of N on A is non-trivial, vanishing quadratically as $A \to 0$. The partial probability of B is Gaussian (cf (3.17)): since this result is not surprising no numerical results will be given for this statistic.

To test the statistics (4.1) and (4.2), the parameter-dependent matrix model described in § 2 was programmed on a computer, using a random number generator to provide a discrete simulation of the white noise sources, $W_{ij}(X)$. The eigenvalues of the resulting random matrices were evaluated at small intervals ΔX. Avoided crossings were identified by searching for the discrete values of X at which the separation of two eigenvalues had a local minimum. If two eigenvalues $E^{\pm}$ had a local minimum separation at $X_n = n\Delta X$, the parameters X_0, A, $\Delta\varepsilon$ were calculated using the following equations, where $\Delta n = (E^+(X_n) - E^-(X_n))^2$:

$$X_0 = X_n - [\Delta X(\Delta_{n-1} - \Delta_{n-1})/2(\Delta_{n+1} + \Delta_{n-1} - 2\Delta_n)] \tag{4.3}$$

$$A = [(\Delta_{n+1} - \Delta_{n-1})/4(X_0 - X_n)\Delta X]^{1/2} \tag{4.4}$$

$$\Delta\varepsilon = [\Delta_n - A^2(X_0 - X_n)^2]^{1/2}. \tag{4.5}$$

These expressions are easily derived from the standard form for an avoided crossing (3.1). The value of A is only meaningful if $\Delta\varepsilon$ is small and the avoided crossing is well separated from its neighbours. Only avoided crossings between states in the central region of the spectrum were included, where the density of states is close to its maximum value (cf (2.3)):

$$n_0 = \sqrt{N}/\pi\mu. \tag{4.6}$$

In the numerical experiments, I used random matrices of dimension $N = 31$, with variance parameters $\sigma = \mu = 1$, and only avoided crossings for which the lower eigenvalue was between the 10th and the 22nd (inclusive) were included in the statistics. The parameter X was varied from 0 to 200, enabling several thousand avoided crossings to be identified. Results for F, the number of avoided crossings per unit length with gap size less than $\Delta\varepsilon$, are shown in table 1. There is good agreement with the predicted values, even for quite large values of $\Delta\varepsilon$, where the theory is expected to break down. When $n_0\Delta\varepsilon \ll 1$, the theoretical values overestimate F by a few per cent. This is probably due to the fact that the density of states is not constant, and the maximum value, given by (4.6), was used to calculate F_{pred}. The probability distribution of A is compared with the theoretical prediction in figure 2. Only avoided crossings for which $n_0\Delta\varepsilon < 0.3$ were included (a sample of 1557). Again, there is good agreement with the theoretical prediction.

Table 1. Comparison of computed values of F, the number of avoided crossings per unit length with gap sizes less than $\Delta\varepsilon$, with the theoretical value F_{pred} calculated from (4.1). The dimension of the matrix was $N = 31$ and the variance parameters were $\mu = \sigma = 1$; n_{cr} is the total number of avoided crossings for which the lower level lay between the 10th and the 22nd between $X = 0$ and $X = 200$.

$n_0\Delta\varepsilon$	n_{cr}	F	F_{pred}
0.05	235	0.098	0.116
0.1	499	0.208	0.233
0.2	1069	0.445	0.465
0.3	1557	0.649	0.698
0.5	2410	1.004	1.163
0.8	3435	1.431	1.861

5. Concluding remarks

The results derived in § 3 are applicable to many other systems besides the GOE random matrix model: they should apply to most one-parameter families of quantum systems without any symmetries or conserved quantities. In order to apply the theory to other systems, it is necessary to know σ^2, the variance of the matrix elements of $\partial H/\partial x$, as well as the density of states n_0. One way to estimate σ is empirically from a set of values of $\mathrm{d}E_n/\mathrm{d}X$: from (2.1), we see that the variance of $\mathrm{d}E_n/\mathrm{d}X = (\partial H/\partial X)_{nn}$ is equal to $2\sigma^2$. If the system has a classical limit for which the motion is chaotic, it is also possible to calculate σ^2 from a correlation function of the classical motion (Wilkinson 1987).

All of the results described above refer to time-reversal-invariant systems with GOE spectral statistics. If the system does not have time-reversal invariance (due to the presence of a magnetic field), the energy level statistics are those of the Gaussian unitary ensemble (GUE). In this ensemble the off-diagonal matrix elements are complex, with their real and imaginary parts independently Gaussian distributed, each with variance $\frac{1}{2}\sigma^2$, and the diagonal elements are independently Gaussian distributed with variance σ^2 (Porter 1965). Because the off-diagonal matrix elements are complex there

is stronger level repulsion, and the density of avoided crossings is proportional to $\Delta\varepsilon$ for small $n_0\Delta\varepsilon$:

$$N(A, B, \Delta\varepsilon)\,dA\,dB\,d\Delta\varepsilon = P[B]\,dB\frac{\pi\sqrt{\pi}}{12}\frac{n_0^3\Delta\varepsilon}{\sigma^3}A^3\exp(-A^2/4\sigma^2)\,dA\,d\Delta\varepsilon \tag{5.1}$$

where

$$P[B]\,dB = (2\pi)^{-1/2}\sigma^{-1}\exp(-B^2/2\sigma^2)\,dB. \tag{5.2}$$

This result can be derived by a simple adaptation of the method used in § 3.

Acknowledgment

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Appendix

We wish to choose the smoothing function $f(X)$ in (2.4) so that the variances of the off-diagonal matrix elements and their derivatives are respectively μ^2 and σ^2. These variances are easily obtained from the correlation function $C(\Delta X)$:

$$\begin{aligned} C(\Delta X) &= \langle H_{ij}(\Delta X)H_{ij}(0)\rangle \\ &= \mu^2\int_{-\infty}^{\infty}dX_1\int_{-\infty}^{\infty}dX_2 f(\Delta X - X_1)f(-X_2)\langle W_{ij}(X_1)W_{ij}(X_2)\rangle \\ &= \mu^2\int_{-\infty}^{X}dX' f(X-X')f(-X'). \end{aligned} \tag{A1}$$

By definition, $C(0)$ is the variance of H_{ij}. The variance of the derivative can be calculated as follows:

$$\frac{dH_{ij}}{dX} = \lim_{\Delta X\to 0}\left(\frac{H_{ij}(X+\Delta X)-H_{ij}(X)}{\Delta X}\right) \tag{A2}$$

$$\begin{aligned} \left\langle\left(\frac{dH_{ij}}{dX}\right)^2\right\rangle &= \lim_{\Delta X\to 0}\frac{1}{\Delta X^2}\{\langle H_{ij}^2(\Delta X)+H_{ij}^2(0)-2H_{ij}(\Delta X)H_{ij}(0)\rangle\} \\ &= \lim_{\Delta X\to 0}\frac{2}{\Delta X^2}\{\mu^2 - C(\Delta X)\} = \sigma^2. \end{aligned} \tag{A3}$$

The correlation function must therefore satisfy the equations

$$C(0) = \mu^2 \tag{A4}$$

$$C'(0) = 0 \tag{A5}$$

$$C''(0) = -\sigma^2. \tag{A6}$$

Using the filter function given by (2.6) and evaluating the correlation function using (A1), we find

$$C(\Delta X) = \frac{\mu^2 a^2}{4b^5}\exp(-b\Delta X)(3+3b\Delta X+b^2\Delta X^2). \tag{A7}$$

This immediately satisfies (A5), and also satisfies (A4) and (A6) with the following choice of constants:

$$a = 2.3^{3/4}(\sigma/\mu)^{5/2} \qquad b = \sqrt{3}\,\sigma/\mu. \tag{A8}$$

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