Singularities in the spectra of random matrices

Paul N. Walker[a)]
Department of Physics and Applied Physics, John Anderson Building, University of Strathclyde, Glasgow, G4 0NG, Scotland, United Kingdom

María José Sánchez[b)] and Michael Wilkinson[c)]
Université Pierre et Marie Curie, Institut Henri Poincaré, 11 Rue Pierre et Marie Curie, Paris Cedex 05, France

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We consider singularities of the set of energy levels $E_n(\mathbf{X})$ of a quantum Hamiltonian, obtained by varying a set of d parameters $\mathbf{X}=(X_1,..,X_d)$. Singularities such as minima, degeneracies, branch points, and avoided crossings can play an important role in physical applications. We discuss a general method for counting these singularities, and apply it to a random matrix model for the parameter dependence of energy levels. We also show how the density of avoided crossing singularities is related to a non-analyticity of a correlation function describing the energy levels. © *1996 American Institute of Physics.* [S0022-2488(96)01810-5]

I. INTRODUCTION

It is now widely accepted that random matrices provide an excellent model for statistical properties of the spectra of quantum systems for which the energy levels cannot be determined analytically:[1,2] random matrix models have been successfully applied to disordered solids, classically chaotic systems, and many body problems. There are many contexts in which families of Hamiltonians depending smoothly on a set of parameters are of physical importance, for example the parameters could represent the positions of atomic nuclei in the Hamiltonian for the electrons in a molecule, or the Bloch wavevectors of an electron in a periodic potential. Recently the random matrix approach has been extended to describe statistics which characterize the parameter dependence of energy levels.[3–9] One approach to analyzing the parameter dependence is to consider correlation functions; an example which has received attention[6–8] is the correlation function $C(X)$ of the derivatives of energy levels $E_n'=dE_n/dX$:

$$C(X)=\langle E_n'(X+X_0)E_n'(X_0)\rangle.\neg \tag{1.1}$$

An alternative approach is to examine various types of singularity in the spectrum, such as degeneracies[9,10] (where a pair of energy levels become equal at some real valued point in the parameter space), branch points[8] (where energy levels become degenerate at complex parameter values), and avoided crossings[3] (characteristic structures where energy levels come close to degeneracy). These singularities can have direct physical consequences, in determining various aspects of the breakdown of the adiabatic theorem,[11–14,3] and discontinuities of the quantized Hall conductance.[15,16,10]

This paper has two objectives. The first is to explain the strategy for calculating the density of singularities in the parameter space; we will present some new calculations of the density of singularities, as well as reviewing existing results. The second objective is to discuss the implications of these results for the calculation of correlation functions such as (1.1). Guaneri *et al.*[8]

[a)]New address: Laboratoire de Physique des Solides, Bâtiment 510, Université Paris-Sud, 91405 Orsay Cedex, France.
[b)]Permanent address: Division de Physique Théorique, Institut de Physique Nucléaire, 91406 Orsay Cedex, France.
[c)]Permanent address: Department of Physics and Applied Physics, John Anderson Building, University of Strathclyde, Glasgow, G4 0NG, Scotland, United Kingdom.

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demonstrated that the existence of branch point singularities in the spectrum implies that correlation functions such as $C(X)$ have a non-analytic behavior at $X=0$. We will show how the leading order non-analytic part of this function is obtained from the density of singularities.

This paper is organized as follows. In Sec. II we discuss parameter dependent generalizations of the standard random matrix models. In Sec. III we describe the approach to counting densities of singularities of random functions, using the density of minima as an example. In Sec. IV we review the known results on the density of various types of singularity, and their physical applications. Some of the results in Sec. IV are new, and of these the density of degeneracies for the GUE and GSE ensembles are not easily obtained; these calculations are explained in Sec. V and in an Appendix. Finally in Sec. VI we discuss the implications of the results given in Sec. IV for correlation functions such as (1.1).

In this paper we will discuss a variety of different probability distributions. To avoid naming a multiplicity of different functions describing these distributions, we will introduce the notational convention that $dP=P[X]dX$ is a probability measure for the quantity X.

II. PARAMETER DEPENDENT RANDOM MATRICES

The most fundamental random matrix models are the Gaussian ensembles introduced by Porter and Dyson. These are constructed from real symmetric matrices $\tilde{H}^{(S)}$ and real antisymmetric matrices $\tilde{H}_k^{(A)}$ with independent Gaussian distributed elements; the variance of the ijth element of these matrices is, respectively, $1\pm\delta_{ij}$. There are three Gaussian ensembles, invariant under orthogonal, general unitary, and ''symplectic'' unitary transformations,[1,2] which are constructed from combinations of the symmetric and antisymmetric matrices as follows:

$$[\tilde{H}]_{ij}=\frac{1}{\sqrt{\beta}}\left\{[\tilde{H}^{(S)}]_{ij}\mathbf{e}_0+\sum_{k=1}^{\beta-1}[\tilde{H}_k^{(A)}]_{ij}\mathbf{e}_k\right\}.\neg \tag{2.1}$$

Here $\beta=1,2,4$ for the orthogonal, unitary and symplectic ensembles, respectively, $\mathbf{e}_0$, $\mathbf{e}_1$ are 1, $\sqrt{-1}$, respectively, and the other $\mathbf{e}_k$ are the other bases for the quaternion algebra. In order for these to be useful models for energy level statistics, the dimension N of the matrix should be large.

In order to study singularities of the spectrum, it is necessary to construct a parameter dependent version of these random matrix models. It is convenient to do this in such a way that $\partial\hat{H}/\partial X$ is an independent realization of the same ensemble as $\hat{H}$, and that the distribution of both of these quantities is stationary: this is achieved by writing

$$\hat{H}(X)=\cos X\hat{H}_1+\sin X\hat{H}_2,\neg \tag{2.2}$$

where $\hat{H}_1$ and $\hat{H}_2$ are Hermitean operators represented by independent samples from the same Gaussian symmetry-invariant ensemble defined above. Reference 5 discusses theoretical arguments and numerical results which support the use of (2.2) as a model for parameter dependencies of spectra. In the calculations below, we will require the matrix elements of $d\hat{H}/dX$ in the basis formed by the eigenstates of $\hat{H}$: this is simply an arbitrary unitary transformation of $d\hat{H}/dX$ within the appropriate symmetry class (orthogonal, unitary, or symplectic). Because the Gaussian invariant ensembles are invariant under these unitary transformations, the matrix elements $\partial H_{nm}\equiv\langle\phi_n|d\hat{H}/dX|\phi_m\rangle$ have the same statistical properties as those of the matrix $d\hat{H}/dX$.

In order to compare a random matrix model with the spectrum of a ''real'' physical system in the neighborhood of energy E, we must scale energy levels of the system so that the density of states $\rho(E)$ corresponds to that of the random matrix model. In a parameter dependent system, it is also necessary to adjust another parameter, describing the sensitivity of the energy levels of the system to perturbations: the natural choice is to use either the variance of the off-diagonal matrix elements of $d\hat{H}/dX$ in the eigenbasis,

$$\sigma^2(E)=\langle|\partial H_{nm}|^2\rangle_{\substack{E_n\sim E_m\sim E\\ n\neq m}},\neg \tag{2.3}$$

or the variance of dE_n/dX: these are related by

$$\mathrm{var}\left[\frac{dE_n}{dX}\right]=\frac{2}{\beta}\sigma^2.\neg \tag{2.4}$$

Equation (2.4) follows from the definition (2.1) for the Gaussian random matrix models, and there are several arguments suggesting that it should also hold for complex quantum systems.[17,18] For the random matrix ensemble (2.2), we have $\sigma=1$.

The model (2.2) can be extended to systems with d parameters in several ways; the simplest is to use $2d$ independent realizations of the random matrices, and write

$$\hat{H}(\mathbf{X})=\sum_{i=1}^{d}\ \cos X_i\hat{H}_{2i-1}+\ \sin X_i\hat{H}_{2i}.\neg \tag{2.5}$$

Now the sensitivity of energy levels to the parameters X_i can be characterized by defining a set of parameters C_{ij} which generalize (2.3):

$$C_{ij}=\langle\partial_i H^*_{nm}\partial_j H_{nm}\rangle_{\substack{E_n\sim E_m\sim E\\ n\neq m}},\neg \tag{2.6}$$

where $\partial_i H_{nm}\equiv\langle\phi_n|\partial\hat{H}/\partial X_i|\phi_m\rangle$. A change of variables makes the parameter dependence of the energy levels resemble that of the model (2.5). In the many-parameter case the parameter σ characterizing the sensitivity of energy levels is naturally defined in terms of the Jacobean of this transformation: noting that for (2.5) we have $C_{ij}=\delta_{ij}$, the natural definition is

$$\sigma^2=(\det[\widetilde{C}])^{1/d},\neg \tag{2.7}$$

where $\widetilde{C}$ is a matrix with elements C_{ij}. In order to use the parametrized random matrix models, both the density of states ρ and the sensitivity parameter σ must be estimated. This can always be done numerically calculating an average over energy levels. For systems which exhibit semiclassical behavior, ρ can be estimated using the Weyl formula,[19] and σ^2 can be estimated from the classical correlation function of $\partial H/\partial X$.[20]

III. COUNTING SINGULARITIES

The method which we use for calculating the density of singularities can be viewed as an extension of one described by Rice,[21] who gives an expression for the frequency of zero crossings of a random function $f(x)$, for which the joint probability density of the function and its derivative f' is known. If $\mathscr{D}^{(0)}$ is the density of zeros of the function, the probability of finding a zero in a short interval of length $[x_0,x_0+\delta x]$ at a randomly chosen point x_0 is $\delta P=\mathscr{D}^{(0)}\delta x$. If the point x_0 happens to be close to a zero, the distance from x_0 to this zero crossing is approximately $-f(x_0)/f'(x_0)$, and the probability of the zero crossing lying within δx of x_0 is

$$\delta P\sim\int_{-\infty}^{\infty}df\int_{-\infty}^{\infty}df'\,P[f,f']\chi\left(\frac{-f}{f'\delta x}\right),$$
$$\chi(x)=\begin{cases}1,\neg & 0<x<1,\\ 0,\neg & 0>x>1.\end{cases} \tag{3.1}$$

Dividing by δx and taking the limit $\delta x\to 0$ gives

$$\mathscr{D}^{(0)}=\int_{-\infty}^{\infty}df\int_{-\infty}^{\infty}df'\,P[f,f']\delta\left(\frac{f}{f'}\right)=\int_{-\infty}^{\infty}df'|f'|P[0,f'].\neg \tag{3.2}$$

The same approach is used to determine the density of any point singularity: we use the known statistics of the function to calculate the probability of finding a singularity in a small element centered on a randomly chosen test point, and equate this to the density of singularities multiplied by the volume of the element.

As an elementary example, we can use (3.2) to determine the density of minima $\mathscr{D}^{(\min)}$ of $E_n(X)$ for the random matrix model (2.2). The density of minima might find physical applications, for example in determining the number of possible energetically stable configurations of complex molecules which can be obtained by varying configuration of the nuclei.

The first and second derivatives of $E_n(X)$,

$$E_n'=\frac{dE_n}{dX}=\partial H_{nn},\neg\quad E_n''=\frac{d^2E_n}{dX^2}=2\sum_{m\neq n}\frac{|\partial H_{nm}|^2}{(E_n-E_m)}-2E_n,\neg \tag{3.3}$$

are independent, because they depend upon different matrix elements. We denote the distributions of the first two derivatives by $P[E']$ and $P[E'']$, respectively. The first derivative E' is Gaussian distributed with variance $2\sigma^2/\beta$, and with a mean value which is zero for the model (2.2), but which may have a non-zero value $\langle E'\rangle$ in physical applications. The distribution of the second derivative is difficult to calculate: when the matrix dimension N is large, an excellent approximation[22] is

$$P[E'']=\frac{C_\beta}{[a_\beta^2+E''^2]^{(\beta+2)/2}},\neg \tag{3.4}$$

which is also an exact result for the GUE in the limit $N\to\infty$.[23] The constants C_β are given in Refs. 4,5,

$$C_1=2\pi^2\rho^2\sigma^4,\neg\quad C_2=2^4\pi^2\rho^3\sigma^6,\neg\quad C_4=2^8\pi^4\rho^5\sigma^{10}/3,\neg \tag{3.5}$$

and the a_β are then determined by normalizing the distribution: we find $a_1=2\pi\rho\sigma^2$ and $a_1=a_2=a_4$. The density of minima can now be calculated by using (3.2) to calculate the density of zeros of $E_n'(X)$, and dividing by two because half of the extrema of $E_n(X)$ are maxima:

$$\mathscr{D}_\beta^{(\min)}=P[E'=0]\int_0^\infty dE''|E''|P[E'']=C_\beta^{(\min)}\rho\sigma\,\exp\left[\frac{-\beta\langle E'\rangle^2}{4\sigma^2\neg}\right],\neg \tag{3.6}$$

with dimensionless constants

$$C_1^{(\min)}=\frac{\sqrt{\pi}}{2},\neg\quad C_2^{(\min)}=\sqrt{\frac{2}{\pi}},\neg\quad C_4^{(\min)}=\frac{4}{3\sqrt{\pi}}.\neg \tag{3.7}$$

These results are exact for the GUE in the limit $N\to\infty$, and at least a very good approximation for the GOE and GSE.

IV. REVIEW OF RESULTS ON DENSITY OF SINGULARITIES

Below we discuss the various other types of singularity of the spectrum which are of interest and their physical significance, and review the existing results on their density. All of the results are exact for the random matrix models introduced in Sec. II in the limit $N\to\infty$.

A. Degeneracies

A degeneracy occurs when two or more energy levels are equal for some real valued point in parameter space; in practice we will only be interested in degeneracies between pairs of levels, because higher order degeneracies have a higher codimension. Generically, two parameters must be varied in a family of real symmetric matrices to create a degeneracy, three parameters in a family of Hermitean matrices, and five parameters in a family of quaternion symmetric matrices.[24] We will therefore consider the density of degeneracies in the model (2.5) with $d=2,3,5$ for the GOE, GUE and GSE versions, respectively.

An interesting example of the importance of degeneracies is given by Simon,[15] who shows that the Chern integers describing the quantized Hall conductance[16] change, typically by ± 1, at degeneracies. Degeneracies can also enable other invariant quantities to change; for example the center of symmetry associated with Wannier functions of a Bloch band can change discontinuously when the band touches a neighboring band at some point in the Brillouin zone.

The density of degeneracies for the parametrized ensembles is defined in a space of $\beta+1$ parameters, and their density is

$$\mathscr{D}_\beta^{(\mathrm{deg})} = C_\beta^{(\mathrm{deg})} (\rho\sigma)^{\beta+1}, \tag{4.1}$$

with dimensionless prefactors

$$C_1^{(\mathrm{deg})} = \frac{\pi}{3}, \quad C_2^{(\mathrm{deg})} = \frac{2\sqrt{\pi}}{3}, \quad C_4^{(\mathrm{deg})} = \frac{16\sqrt{2}\,\pi^{3/2}}{45}; \tag{4.2}$$

$C_1^{(\mathrm{deg})}$ was derived in Ref. 9 and $C_2^{(\mathrm{deg})}$ was quoted in Ref. 10 without a full derivation. An estimate consistent with (4.1) was given in an earlier paper[25] for the special case of billiards, without an accurate value of the prefactor. The derivations of $C_2^{(\mathrm{deg})}$ and $C_4^{(\mathrm{deg})}$ will be given in Sec. V and in an Appendix, respectively.

In the neighborhood of a degeneracy, the separation $\Delta = E_{n+1} - E_n$ of the degenerating levels is given by the square root of a quadratic form; for example in the case of a system such as the GOE, where the Hamiltonian is real, we can write

$$\Delta^2 = A_{11}\delta X_1^2 + A_{22}\delta X_2^2 + 2A_{12}\delta X_1 \delta X_2 + O(\delta X^3). \tag{4.3}$$

This quadratic form can be defined by the orientation, eccentricity, and size of the elliptical level curves of Δ. For the model (2.5), the orientation of the ellipses is random, and the other parameters are defined by the trace $t = A_{11} + A_{22}$ and determinant $d = A_{11}A_{22} - A_{12}^2$ of the matrix which represents the quadratic form. The joint distribution of the trace and determinant has been calculated:[9] it is

$$P[t,d] = \frac{d}{256\sigma^6} \exp\left(\frac{-t}{8\sigma^2} \right), \tag{4.4}$$

within the physically allowed region $t>0$, $d>0$, $d \leqslant \frac{1}{2}t^2$. Other statistics describing the elliptical contours of Δ can be obtained directly from this simple result; for example the distribution of eccentricity e of the ellipses is

$$P[e] = \left(\frac{2e}{2-e^2} \right)^3. \tag{4.5}$$

The distribution of parameters of the quadratic form for the unitary and symplectic ensembles is not known.

B. Avoided crossings

When a single parameter is varied, energy levels of systems without symmetries never cross,[26] but they can approach each other very closely at events called avoided crossings. When the separation of a pair of energy levels is very small compared to their separation from all of the other levels, the structure of these avoided crossings can be understood using degenerate perturbation theory for a two level system: provided the Hamiltonian is a regular function of parameter in the neighborhood of the near-degeneracy, the levels have a hyperbolic form,

$$E_{\pm}(X) \sim B(X-X_0) \pm \frac{1}{2}\sqrt{\epsilon^2 + A^2(X-X_0)^2}.\neg \tag{4.6}$$

The avoided crossing is characterized by four parameters, the gap ϵ, the difference of the asymptotic slopes A, the mean of the asymptotic slopes B, and the position X_0.

Avoided crossings are physically important because they mediate the breakdown of the adiabatic theorem by Landau-Zener transitions,[11,12,3] and in Sec. VI we will show that they determine the form of singular terms in the expansion of correlation functions such as (1.1).

The density of avoided crossings can be defined as follows: $\mathscr{D}_\beta^{(\mathrm{ac})}(A,B,\epsilon)dAdBd\epsilon dX$ is the expected number of avoided crossings between a given pair of successive levels, in an interval of length dX, for which the slope difference, mean slope, and gap parameters all lie in intervals of widths, respectively, dA, dB, $d\epsilon$, centered on the values A, B, ϵ. This statistic is only meaningful for small values of ϵ, because A and B are only defined for avoided crossings with gaps which are very small compared to the mean level separation $1/\rho$. The avoided crossing density is calculated by exactly the same approach as for the density of degeneracies, although the calculation is somewhat more difficult: the result, obtained in Refs. 3 and 5 is

$$\mathscr{D}_\beta^{(\mathrm{ac})}(A,B,\epsilon)dAdBd\epsilon = P[B]dBC_\beta^{(\mathrm{ac})}(\rho/\sigma)^{\beta+1}\epsilon^{\beta-1}d\epsilon A^{\beta+1}\ \exp[-\beta A^2/8\sigma^2]dA,\neg \tag{4.7}$$

where $P[B]dB$ is a Gaussian distribution, with variance σ^2/β, and

$$C_1^{(\mathrm{ac})} = \frac{\pi}{24},\neg \quad C_2^{(\mathrm{ac})} = \frac{\pi^{3/2}}{12},\neg \quad C_4^{(\mathrm{ac})} = \frac{8\pi^{7/2}}{135\sqrt{2}}.\neg \tag{4.8}$$

C. Branch points

Degeneracies between levels of the one parameter model (2.2) can occur for complex values of X; these degeneracies have a branch point structure. The branch points are important because they are used to determine the exponents describing the probability of non-adiabatic transitions.[13,14] Branch points can be identified with a particular pair of levels by considering a closed path in the complex X plane which leaves the real axis and loops around one, and only one, branch point. For all but one of the levels indices n, the energy level $E_n(X)$ is single valued when traced around this path, but one level, E_m say, is continuously transformed into another level $E_{m'}$ when traced around this path. The levels with indices m, m' are connected by the branch point.

We define $\mathscr{D}_\beta^{(\mathrm{br})}(Y,N)dY$ to be the frequency with which we encounter branch points involving the nth level and the level $n+N$, with the imaginary part of the parameter X in an interval of width dY centered on Y.

We have only been able to find the density of branch points for $N=1$ and small Y. Branch points very close to the real axis are associated with avoided crossings with very small values of ϵ: the distance of the branch point from the real axis is ϵ/A. The density of these branch points is obtained immediately from (4.7) and (4.8):

$$\mathscr{D}_\beta^{(\mathrm{br})}(Y,1)=\int_0^\infty dA\int_{-\infty}^\infty dB\int_0^\infty d\epsilon\,\mathscr{D}^{(\mathrm{ac})}(A,B,\epsilon)\,\delta\left(\ Y-\frac{\epsilon}{A}\ \right)$$

$$=C_\beta^{(\mathrm{br})}(\rho\sigma)^{\beta+1}Y^{\beta-1},\neg \tag{4.9}$$

with dimensionless constants

$$C_1^{(\mathrm{br})}=\frac{4\pi}{3},\neg\quad C_2^{(\mathrm{br})}=\frac{16\pi^{3/2}}{3},\neg\quad C_4^{(\mathrm{br})}=\frac{2^{10}\pi^{7/2}}{45\sqrt{2}}.\neg \tag{4.10}$$

Guarneri *et al.*[8] gave an argument for an expression of the form (4.9), but did not obtain the prefactors (4.10).

V. DENSITY OF DEGENERACIES

We now discuss how to determine the density of degeneracies. This has already been described in detail for the Gaussian orthogonal ensemble,[9] and the result for the Gaussian unitary ensemble has also been quoted in an earlier paper.[10] Here we discuss the GUE case in detail, presenting details of the calculation which were omitted in Ref. 10; the calculation for the GSE case is similar, and is discussed in an Appendix.

Following the approach introduced in Sec. III, we select an arbitrary point in parameter space $\mathbf{X}_0$. We assume that this point is close to a degeneracy between levels with indices n and $n+1$. In the neighborhood of this point we represent the Hamiltonian in the basis formed by the eigenfunctions $|\psi_n(\mathbf{X}_0)\rangle$ at $\mathbf{X}_0$, and apply two-state degenerate perturbation theory. The separation of the nearly degenerate levels at a nearby position $\mathbf{X}=\mathbf{X}_0+\delta\mathbf{X}$ is

$$E_{n+1}-E_n\sim\sqrt{\left[\Delta+\sum_i\ (\partial_i H_{n+1\,n+1}-\partial_i H_{nn})\,\delta X_i\right]^2+4\left|\sum_i\ \partial_i H_{nn+1}\delta X_i\right|^2}\quad,\neg \tag{5.1}$$

where $\Delta=E_{n+1}(\mathbf{X}_0)-E_n(\mathbf{X}_0)$. Within this approximation the degeneracy occurs when the discriminant (5.1) vanishes, at a displacement $\delta\mathbf{X}$ from $\mathbf{X}_0$. The components δX_i of this displacement are given by solving a system of linear equations:

$$\sum_{j=1}^3 M_{ij}\delta X_j=\Delta\,\delta_{1j}\,,\neg \tag{5.2}$$

where the elements of the 3×3 matrix $\widetilde{M}=\{M_{ij}\}$ are

$$\begin{aligned} M_{1j}&=\partial_j H_{n+1\,n+1}-\partial_j H_{nn}\,,\\ M_{2j}&=2\ \mathrm{Re}[\partial_j H_{nn+1}],\neg\quad M_{3j}=2\ \mathrm{Im}[\partial_j H_{nn+1}]. \end{aligned} \tag{5.3}$$

Note that the M_{ij} are elements of a real, non-symmetric, random matrix $\widetilde{M}$ with statistically independent elements, all of which are identically Gaussian distributed, with variance $2\sigma^2$ and mean 0.

The distance from the reference point to the degeneracy, $R=|\delta\mathbf{X}|$, is proportional to Δ: we write $R=\Delta f$ where

$$f^2=\sum_{i=1}^3\ [(\widetilde{M}^{-1})_{i1}]^2.\neg \tag{5.4}$$

The probability $P[R]$ that the nearest degeneracy exists at a small distance R can then be written, by analogy with (3.2),

$$P[R]=\int_0^\infty df\int_0^\infty d\Delta P[f]P[\Delta]\delta(R-f\Delta), \tag{5.5}$$

where $P[f]$ is the probability distribution for f, and $P[\Delta]$ is the distribution of neighboring energy level separations: these quantities are independent because of the statistical independence of $\hat{H}$ and $\partial_i\hat{H}$ (note that Δ depends only upon $\hat{H}$ whereas f depends only upon the matrix elements $\partial_i H_{nm}$). The distribution $P[\Delta]$ is the well known level spacing distribution.[1,2] When R is small, the Dirac delta function only supports small values of Δ, for which the level spacing distribution is known analytically[2] in the limit $N\to\infty$:

$$P[\Delta]d\Delta=\left[\frac{1}{3}\pi^2\rho^3\Delta^2+O(\Delta^3)\right]d\Delta,\neg \tag{5.6}$$

where ρ is the density of states. Performing the integrals in (5.5) gives

$$P[R]=\left[\frac{1}{3}\pi^2\rho^3\langle f^{-3}\rangle R^2+O(R^3)\right]dR.\neg \tag{5.7}$$

The expected number of degeneracies in a spherical shell of radius R and thickness dR is $4\pi\mathscr{D}_2^{(\mathrm{deg})}R^2dR$; comparing this with (5.7) gives

$$\mathscr{D}_2^{(\mathrm{deg})}=\frac{1}{12}\pi\rho^3\langle f^{-3}\rangle.\neg \tag{5.8}$$

It remains to evaluate the integral $I=\langle f^{-3}\rangle$, by averaging over the probability density

$$dP=P[\tilde{M}]d\tilde{M}=P[M_{11},M_{12},\ldots,M_{33}]\prod_{ij}dM_{ij}=A\exp\left[-\frac{\mathrm{tr}(\tilde{M}^T\tilde{M})}{4\sigma^2}\right]d\tilde{M},\neg \tag{5.9}$$

where A is a normalization factor. To facilitate the calculation of the average, the non-symmetric real matrix $\tilde{M}$ is decomposed into a product of two orthogonal matrices $\tilde{O}_1$, $\tilde{O}_2$, and a diagonal matrix $\tilde{D}$:

$$\tilde{M}=\tilde{O}_1^T\tilde{D}\tilde{O}_2.\neg \tag{5.10}$$

This gives a useful simplification of the expression for f:

$$f^2=\sum_{i=1}^3[(\tilde{O}_1^T\tilde{D}\tilde{O}_2)^{-1}]_{i1}^2=\sum_{i=1}^3[\tilde{O}_2^T\tilde{D}^{-1}\tilde{O}_1)_{i1}]^2=\sum_{i=1}^3\lambda_i^{-2}(\tilde{O}_1)_{i1}^2,\neg \tag{5.11}$$

where λ_i is the ith diagonal element of $\tilde{D}$. Also, the trace in (5.9) takes on a simple form when we use (5.10):

$$\mathrm{tr}(\tilde{M}^T\tilde{M})=\mathrm{tr}(\tilde{D}^2)=\sum_{i=1}^3\lambda_i^2.\neg \tag{5.12}$$

We can now calculate $\langle f^{-3}\rangle$ by transforming from the coordinates $\{M_{ij}\}$ to a set of coordinates consisting of the three diagonal elements of $\tilde{D}$, and two sets of three coordinates

$\alpha=\{\alpha_1,\alpha_2,\alpha_3\}$ and $\beta=\{\beta_1,\beta_2,\beta_3\}$ which parametrize the orthogonal matrices $\widetilde{O}_1$ and $\widetilde{O}_2$, respectively. The Jacobian J of the coordinate transformation is defined by

$$d\widetilde{M}=Jd\alpha_1 d\alpha_2 d\alpha_3 d\beta_1 d\beta_2 d\beta_3 d\lambda_1 d\lambda_2 d\lambda_3,\neg \tag{5.13}$$

where $J=|\det\widetilde{j}\,|$ and $\widetilde{j}$ is composed of three, 9×3 blocks:

$$\widetilde{j}=\left(\frac{\partial\widetilde{M}}{\partial\lambda}\,\middle|\,\frac{\partial\widetilde{M}}{\partial\alpha}\,\middle|\,\frac{\partial\widetilde{M}}{\partial\beta}\right).\neg \tag{5.14}$$

In the first block, the elements of the type $\partial M_{ij}/\partial\lambda_k$ are independent of the λ_i. In the second block the elements $\partial M_{ij}/\partial\alpha_k$ are linear in the λ_i; the same applies for the third block. Expanding out the determinant, we find that all the terms which contribute to J are 6th degree polynomials in the λ_i. Furthermore, If $\lambda_i=\pm\lambda_j$ for any i,j, then there exists at least one coordinate for the orthogonal matrices $\widetilde{O}_1$, $\widetilde{O}_2$ which does not affect the matrix $\widetilde{M}$. This implies that the Jacobian J must vanish whenever $\lambda_i=\pm\lambda_j$. These observations lead to a unique form for the Jacobian,

$$J=g(\alpha)g(\beta)\prod_{\substack{i,j=1\\ i>j}}^{3}|\lambda_i^2-\lambda_j^2|,\neg \tag{5.15}$$

where $g(\alpha)d\alpha_1 d\alpha_2 d\alpha_3$ is an invariant measure for the orthogonal group. The probability measure in the transformed coordinates is therefore

$$dP=Ag(\alpha)g(\beta)\prod_{\substack{i,j=1\\ i>j}}^{3}|\lambda_i^2-\lambda_j^2|\exp\left[-\frac{1}{4\sigma^2}\sum_{k=1}^{3}\lambda_k^2\right]\prod_{i=1}^{3}d\alpha_i d\beta_i d\lambda_i.\neg \tag{5.16}$$

We can now use (5.11) and (5.16) to evaluate $\langle f^{-3}\rangle$. The three elements $(\widetilde{O}_1)_{i1}$ in (5.11) are components of a unit vector with random direction, and can easily be represented using polar coordinates θ, ϕ. The required average is then

$$\langle f^{-3}\rangle=I_1/I_2,$$

$$I_1=\int d\lambda P[\lambda]\int_0^{\pi}d\theta\,\sin\,\theta\int_0^{2\pi}d\phi(\lambda_1^{-2}\cos^2\,\theta+\lambda_2^{-2}\sin^2\,\theta\sin^2\,\phi+\lambda_3^{-2}\sin^2\,\theta\cos^2\,\phi)^{-3/2}$$

$$I_2=\int d\lambda P[\lambda]\int_0^{\pi}d\theta\,\sin\,\theta\int_0^{2\pi}d\phi, \tag{5.17}$$

where $P[\lambda]$ is the product of the polynomial and exponential in (5.16). After performing the integrals over θ and ϕ, we find

$$\langle f^{-3}\rangle=\frac{\sqrt{8}\sigma^3\mathcal{I}(1,\frac{1}{2},3)}{\mathcal{I}(\frac{1}{2},\frac{1}{2},3)},\neg \tag{5.18}$$

where the $\mathcal{I}(\alpha,\gamma,n)$ are integrals obtained from results derived by Selberg[27] and Aomoto,[28] quoted by Mehta,[2]

$$\mathscr{I}(\alpha,\gamma,n)=\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\prod_{i=1}^{n}|x_i|^{2\alpha-1}\prod_{1\leqslant j<i\leqslant n}|x_i^2-x_j^2|^{2\gamma}\exp\left[\frac{-x_i^2}{2}\right]dx_i$$

$$=2^{\alpha n+\gamma n(n-1)}\prod_{j=1}^{n}\frac{\Gamma(1+\gamma j)\Gamma(\alpha+\gamma(j-1))}{\Gamma(1+\gamma)}.\neg \tag{4.29}$$

We find $\mathscr{I}(1,\frac{1}{2},3)=96$, $\mathscr{I}(\frac{1}{2},\frac{1}{2},3)=24\sqrt{2\pi}$, so that $\langle f^{-3}\rangle=8\sigma^3/\sqrt{\pi}$. The density of degeneracies is therefore $\mathscr{D}_2^{(\mathrm{deg})}=\frac{2}{3}\sqrt{\pi}\rho^3\sigma^3$.

VI. SINGULARITIES OF CORRELATION FUNCTIONS

Now we discuss how the singularities of the energy levels are related to singularities of the correlation function $C(X)$ defined in (1.1). Our contribution builds upon work of Guarneri *et al.*,[8] who showed that the Fourier transform of $C(X)$ has a power law decay as $|k|\to\infty$:

$$\widetilde{C}(k)\sim\frac{\alpha_\beta\sigma}{\rho}\left(\frac{\rho\sigma}{|k|}\right)^{\beta+2},\neg \tag{6.1}$$

where we will define the Fourier transform $\widetilde{f}(k)$ of $f(x)$ as follows:

$$\widetilde{f}(k)=\int_{-\infty}^{\infty}dx f(x)\exp[ikx].\neg \tag{6.2}$$

Guarneri *et al.* were not able to determine the coefficients α_β; we will show how they can be obtained using the results of Sec. IV B. They showed that the power law decay is caused by avoided crossings with small values of the gap parameter ϵ, and deduced that the algebraic decay of $\widetilde{C}(k)$ implies that $C(X)$ has a non-analytic behavior at $X=0$. Using the generalized Fourier transform pairs,[29]

$$\widetilde{f}(k)=\frac{1}{|k|^3}\Leftrightarrow f(x)=\frac{1}{2\pi}x^2\left(\log|x|+\gamma-\frac{3}{2}\right),\neg \tag{6.3a}$$

$$\widetilde{f}(k)=\frac{1}{k^4}\Leftrightarrow f(x)=\frac{1}{12}|x|^3,\neg \tag{6.3b}$$

$$\widetilde{f}(k)=\frac{1}{k^6}\Leftrightarrow f(x)=-\frac{1}{240}|x|^5,\neg \tag{6.3c}$$

it can be seen that (6.1) implies the existence of non-analytic terms in the expansion of the correlation function about $X=0$. Expressed in terms of the natural dimensionless variable $x=\rho\sigma X$, the behaviour of $C(x)$ up to and including the leading non-analytic term is

$$C(x)=2\sigma^2[1+\gamma_1|x|^2\log|x|+\cdots]\quad(\mathrm{GOE}),\neg \tag{6.4a}$$

$$C(x)=\sigma^2[1+C_2^{(2)}x^2+\gamma_2|x|^3+\cdots]\quad(\mathrm{GUE}),\neg \tag{6.4b}$$

$$C(x)=\tfrac{1}{2}\sigma^2[1+C_4^{(2)}x^2+C_4^{(4)}x^4+\gamma_4|x|^5+\cdots]\quad(\mathrm{GSE}).\neg \tag{6.4c}$$

The coefficients of the power series expansion are obtained by a straightforward application of perturbation theory: the quadratic terms were calculated by Simons and Altshuler,[6] and take the values $C_2^{(2)}=-2\pi^2$ and $C_4^{(2)}=-\frac{4}{3}\pi^2$, respectively; the coefficient $C_4^{(4)}$ could also be determined by the same method. The higher order coefficients of the power series expansion diverge because of the effects of small denominators. We will now calculate the coefficients α_β in (6.1), enabling the coefficients γ_β of the singular terms to be identified.

We will find it convenient to assume that the energy levels are periodic in X, with period L, so that the energy level $E_n(X)$ can be expanded as a Fourier series:

$$E_n(X)=\sum_{m=-\infty}^{\infty} a_m \exp\left[\frac{2\pi i m X}{L}\right]. \tag{6.5}$$

Later we will consider the limit $L\to\infty$. The correlation function $C(X)$ will be defined in terms of an average over the length L, which is conveniently expressed in terms of the Fourier coefficients a_m:

$$C(X)=\frac{1}{L}\int_0^L dX' E_n'(X+X')E_n'(X')=\sum_{m=-\infty}^{\infty}\left(\frac{2\pi m}{L}\right)^2 |a_m|^2 \exp\left[\frac{2\pi i m X}{L}\right]. \tag{6.6}$$

For large m, the Fourier coefficients are determined by singularities of $E_n(X)$ closest to the real axis. These are branch points associated with the avoided crossings with small values of the gap parameter ϵ. In order to calculate the effect of these singularities on the Fourier coefficients, we will assume that the second derivative of the energy can be approximated by a sum of contributions from the avoided crossings:

$$E_n''(X)\sim\sum_j (-1)^{P_j} f(X-X_j,A_j,\epsilon_j), \tag{6.7}$$

where A_j, ϵ_j, and X_j are the parameters of the jth avoided crossing. (It is more convenient to use the second derivative, since this approaches zero at $\pm\infty$.) Here the sum runs over all avoided crossings between 0 and L, P_j is zero if the avoided crossing is with a level below, unity for crossing with a level above, and $f(X,A,\epsilon)$ is the second derivative of the energy associated with a single avoided crossing with slope and gap parameters (A,ϵ) at position $X=0$:

$$f(X,A,\epsilon)=\frac{A^2\epsilon^2}{2(A^2X^2+\epsilon^2)^{3/2}}. \tag{6.8}$$

Using (6.7) to estimate the Fourier coefficients a_m, and we find

$$\begin{aligned} a_m &= -\left(\frac{2\pi m}{L}\right)^{-2}\frac{1}{L}\sum_j (-1)^{P_j}\int_0^L dx f(x-X_j,A_j,\epsilon_j) \\ &\sim -\frac{1}{k^2 L}\sum_j (-1)^{P_j}\exp[ikX_j]\tilde{f}(k,A_j,\epsilon_j), \end{aligned} \tag{6.9}$$

where $k=2\pi m/L$, and $\tilde{f}(k,A,\epsilon)$ is the Fourier transform of $f(X,A,\epsilon)$ with respect to X: in the second relation we have assumed that L is sufficiently large that, for all the avoided crossings except those close to $X_j=0$ or $X_j=L$, the errors associated with taking the limits of integration to infinity can be neglected. Using (6.9) to estimate $|a_m|^2$ gives an expression involving a double sum over pairs of avoided crossings. The positions X_j of the narrowly avoided crossings can be

assumed to be random, implying that the average over off-diagonal terms of the double sum containing the phase factor $\exp[ik(X_j - X_{j'})]$ vanishes. We can therefore write

$$|a_m|^2 \sim \frac{1}{k^4 L^2} \sum_j |\tilde{f}(k, A_j, \epsilon_j)|^2$$

$$\sim \frac{2}{k^4 L} \int_0^\infty dA \int_\infty^\infty dB \int_0^\infty d\epsilon \, \mathscr{D}_\beta^{(\mathrm{deg})}(A,B,\epsilon) |\tilde{f}(k,A,\epsilon)|^2, \neg \tag{6.10}$$

where $\mathscr{D}_\beta^{(\mathrm{deg})}$ is the density of avoided crossings defined in Sec. IV B, and the factor of 2 is included because avoided crossings with both the levels above and below must be considered.

The Fourier transform of (6.8) is

$$\tilde{f}(k,A,\epsilon) = k\epsilon K_1(k\epsilon/A), \tag{6.11}$$

where $K_1(x)$ is the Bessel function with imaginary argument.[30,31] In the limit $L \to \infty$ we can approximate the sum in (6.6) as an integral, and using (6.10) we write

$$C(X) = \frac{1}{2\pi} \int_{-\infty}^\infty dk \, \exp[-ikX] \tilde{C}(k), \tag{6.12}$$

$$\tilde{C}(k) = \frac{2}{k^2} \int_0^\infty dA \int_{-\infty}^\infty dB \int_0^\infty d\epsilon \, \mathscr{D}_\beta^{(\mathrm{deg})}(A,B,\epsilon) |\tilde{f}(k,A,\epsilon)|^2$$

$$= \frac{2 C_\beta^{(\mathrm{ac})}}{k^{(\beta+2)}} \left(\frac{\rho}{\sigma} \right)^{\beta+1} \int_0^\infty dA A^{2\beta+3} \exp\left[\frac{-\beta A^2}{8\sigma^2} \right] \int_0^\infty dx x^{\beta+1} |K_1(x)|^2,$$

where we have used (4.7). Using the integral identity[31]

$$\int_0^\infty dx \, x^\nu |K_1(x)|^2 = \frac{2^{\nu-6}(\nu+1)(\nu-1)^3 [\Gamma(\frac{1}{2}(\nu-1))]^4}{\Gamma(\nu+1)}, \neg \tag{6.13}$$

we find that $\tilde{C}(k)$ is in the form (6.1), with dimensionless constants

$$\alpha_1 = 4\pi^3, \quad \alpha_2 = \frac{256\pi^{3/2}}{3}, \quad \alpha_4 = \frac{2^{14}\sqrt{2}\pi^{7/2}}{45}. \neg \tag{6.14}$$

Expressed in terms of the dimensionless variable $x = \rho\sigma X$, the correlation function, up to and including the first singular term, is therefore

$$C(x) = 2\sigma^2 [1 - \pi^2 x^2 \log|x| + \cdots] \quad (\mathrm{GOE}),$$

$$C(x) = \sigma^2 \left[1 - 2\pi^2 x^2 - \frac{64\pi^{3/2}}{9} |x|^3 + \cdots \right] \quad (\mathrm{GUE}), \neg \tag{6.15}$$

$$C(x) = \tfrac{1}{2}\sigma^2 \left[1 - \frac{4\pi^2}{3} x^2 + C_4^{(4)} x^4 + \frac{2048\sqrt{2}\pi^{7/2}}{675} |x|^5 + \ldots \right] \quad (\mathrm{GSE}).$$

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APPENDIX: THE DENSITY OF DEGENERACIES FOR THE GSE

Here we discuss the density of degeneracies $\mathscr{D}_4^{(\mathrm{deg})}$ for a parametrized Gaussian symplectic ensemble. The method employed is the same as that for the GUE, and so can be presented briefly.

The quaternion elements $\mathbf{e}_k$ can be represented by the 2×2 matrices:

$$\mathbf{e}_0=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix},\quad \mathbf{e}_1=\begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix},\quad \mathbf{e}_2=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix},\quad \mathbf{e}_3=\begin{pmatrix}0 & i\\ i & 0\end{pmatrix},\quad \neg \tag{A1}$$

enabling the GSE matrix to be represented by a $2N\times 2N$ real matrix, which has N, 2–fold degenerate eigenvalues: this (Kramer's) degeneracy will be neglected, and we will calculate the density of degeneracies between pairs of these double levels. Five parameters must be varied in order to create these degeneracies.

The condition for a degeneracy between levels n and $n+1$ to be at a distance $\delta\mathbf{X}$ from an arbitrary point can be written in a form analogous to (5.2), where $\widetilde{M}$ is now a 5×5 matrix with elements

$$\begin{aligned} M_{1j}&=[\partial_j\widetilde{H}^{(S)}]_{nn}-[\partial_j\widetilde{H}^{(S)}]_{n+1\,n+1},\\ M_{2j}&=2[\partial_j\widetilde{H}^{(S)}]_{nn+1},\neg\\ M_{ij}&=2[\partial_j\widetilde{H}^{(A)}_{i-2}]_{nn+1},\neg\ \ i=3,4,5. \end{aligned} \tag{A2}$$

Again $\widetilde{M}=\{M_{ij}\}$ is a non-symmetric real matrix with independent, Gaussian distributed elements, with mean value zero; the variance is σ^2 in this case.

The Euclidean length of the vector which solves (5.2) is again written $R=\Delta f$, and following the GUE analysis we find the probability $P[R]dR$ that the nearest degeneracy lies in a shell of thickness dR at distance R. Using the fact that for the GSE, the level spacing distribution is $P[\Delta]d\Delta\sim\frac{16}{135}\pi^4\rho^5\Delta^4 d\Delta$ for $\Delta\rho\ll 1$, $N\gg 1$, we find

$$P[R]\sim\frac{16}{135}\pi^4\rho^5R^4\langle f^{-5}\rangle,\neg \tag{A3}$$

which is valid for small R. The expected number of degeneracies in this shell is $P[R]dR=\frac{8}{3}\pi^2R^4\mathscr{D}_4^{(\mathrm{deg})}dR$ implying that the density of degeneracies for the parameterized GSE is

$$\mathscr{D}_4^{(\mathrm{deg})}=\frac{2}{45}\pi^2\rho^5\langle f^{-5}\rangle.\neg \tag{A4}$$

The integral $I=\langle f^{-5}\rangle$ can be evaluated using the same approach as that used for $\langle f^{-3}\rangle$ in Sec. V, using the decomposition of $\widetilde{M}$ given by (5.10). After some algebra, the original 25 dimensional integral over the M_{ij} is reduced to the quotient of two five dimensional integrals:

$$\langle f^{-5}\rangle = \frac{\sigma^5 \mathscr{I}(1,\frac{1}{2},5)}{\mathscr{I}(\frac{1}{2},\frac{1}{2},5)} = \frac{16\sigma^5}{\sqrt{2\pi}},\neg \tag{A5}$$

where $\mathscr{I}(\alpha,\gamma,n)$ is the integral (5.19). Combining (A4) and (A5), we then find $\mathscr{D}_4^{(\mathrm{deg})} = (16\sqrt{2}\pi^{3/2}/45)\rho^5\sigma^5$.

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