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Parametric statistics of individual energy levels in random Hamiltonians

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We establish a general framework to explore parametric statistics of individual energy levels in disordered and chaotic quantum systems of unitary symmetry. The method is applied to the calculation of the universal *intralevel* parametric velocity correlation function and the distribution of level shifts under the influence of an arbitrary external perturbation.

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Ensembles of random Hamiltonians are used frequently to model properties of diverse physical systems. Although eigenfunction statistics can play an important role in some applications, typically one is interested in the statistics of the spectra $\{\epsilon_i\}$ of such Hamiltonians. Among all the possible statistical ensembles [1], a special role is played by the three invariant Dyson distributions [2]. Characterized by the assumption that the distribution is invariant under, respectively, orthogonal, unitary, and symplectic rotations of the basis, the random matrix theory (RMT) has proved to be remarkably successful in modeling physical systems ranging from nuclear spectra [3] and mesoscopic quantum dots [4] to individual chaotic quantum structures [5].

An important class of problems arises when individual members H of the statistical ensemble undergo parametric evolution according to the rule $H \to H' = H + XV$, where V is a fixed matrix, and X is the strength of the perturbation. Instead of the random variables ϵ_i, one is now confronted with *random functions* $\epsilon_i(X)$ of the external parameter X. Once cast in terms of the rescaled variable $x = X\sqrt{\langle(\partial_X \epsilon_i)^2\rangle}$ (all energies being measured in the units of the mean level spacing Δ), it has been argued [6] that, for a generic perturbation V (see below), the statistical properties of the entire random functions $\epsilon_i(x)$ exhibit the same degree of universality as that of the parent Hamiltonian H. As well as mesoscopic and chaotic quantum structures, universality of the random functions $\epsilon_i(x)$ finds application to a variety of physical systems including step configurations on vicinal surfaces [7], nonintersecting random walkers in one dimension [8], and the world lines of one-dimensional fermions [6].

Beginning with the seminal work of Dyson [9], the statistical properties of the random functions $\{\epsilon_i(x)\}$ have been the subject of numerous investigations [10] (for a review, see, e.g., Ref. [11]). To date, exact analytic expressions have been obtained for the distribution of "local" (in the parameter space) properties such as "level velocities" $\partial_x \epsilon_i(x)$ [6,12,13] and "level curvatures" $\partial_x^2 \epsilon_i(x)$ [14]. At the same time, parametric correlations between the sets $\{\epsilon_i(\bar{x})\}$ and $\{\epsilon_i(\bar{x}+x)\}$ have been explored [6] using field theoretic techniques [11]. As well as establishing the range of universality, explicit expressions for the parametric correlator of the density of states (DOS) and the related level velocity correlation function $\tilde{c}(\omega,x) = \langle \sum_{ij} \partial_{\bar{x}} \epsilon_i(\bar{x}) \partial_{\bar{x}} \epsilon_j(\bar{x}+x) \delta(\epsilon - \epsilon_i(\bar{x})) \delta(\epsilon + \omega - \epsilon_j(\bar{x}+x)) \rangle$ have been inferred.

When the RMT is applied to many-fermion systems, an important distinction arises between two classes of correlation functions: Employing the terminology somewhat loosely, the function $\tilde{c}(\omega,x)$ can be termed "grand canonical" in the sense that the level $\epsilon_j(\bar{x}+x)$ need not be a parametric "descendant" of the level $\epsilon_i(\bar{x})$. Indeed, the definition of $\tilde{c}(\omega,x)$ tracks correlations between $\epsilon_i(\bar{x})$ and a descendant of *any other* level. However, often one is interested in the parametric evolution of the Fermi level or a low-lying excitation in systems with a fixed number of fermions. Inasmuch as such a level can be interpreted as a single particle level of some effective random many-body Hamiltonian, the relevant objects are the canonical correlation functions, exemplified by the *intralevel* velocity correlation function

$$c(x) \equiv \langle \partial_{\bar{x}} \epsilon_i(\bar{x}) \partial_{\bar{x}} \epsilon_i(\bar{x}+x) \rangle. \tag{1}$$

A different perspective is provided by the distribution of single-level shifts

$$p(\omega,x) \equiv \langle \delta(\epsilon_i(\bar{x}+x) - \epsilon_i(\bar{x}) - \omega) \rangle. \tag{2}$$

Apart from their intrinsic interest, it has been argued [4] that the functions $c(x)$ and $p(\omega,x)$ describe parametric correlations of resonant conductance peaks of quantum dots driven into the Coulomb blockade regime and perturbed by a magnetic field or an external gate potential. Similarly, once x is identified with magnetic flux, $c(x)$ coincides with the ensemble-averaged correlation function of single-level persistent currents [11].

To date, studies of parametric correlations of individual energy levels have been limited to numerical investigations. Despite its affinity with $\tilde{c}(\omega,x)$, the intralevel correlation function $c(x)$ (and its canonical counterparts) belongs to a different class of objects. Its analysis presents technical difficulties which are, in part, similar to the challenges encountered in the calculation of the level spacing distribution in nonparametric random matrix ensembles. The latter are known to engage DOS correlations that go beyond the two-point averages presently accessible by field theoretic techniques, and lead to expressions in terms of Fredholm determinants with integrable kernels [2].

The aim of the present paper is to formulate a general framework to explore parametric correlations of *individual* energy levels. In particular, for the *unitary* random matrix ensemble, we will show that

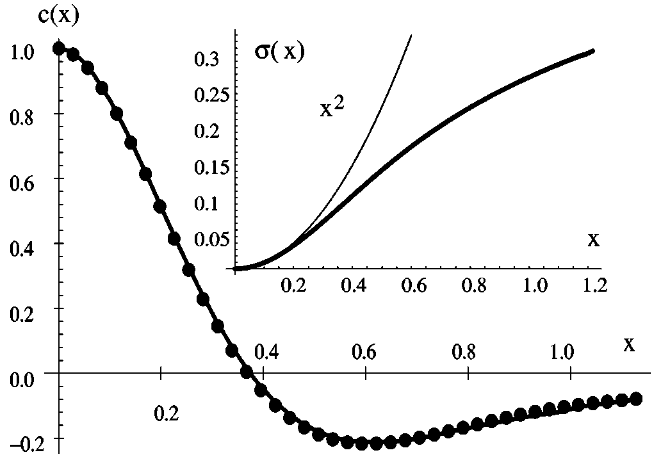

FIG. 1. Level velocity correlation function obtained from Eqs. (3) and (5)–(7) (solid line) vs direct numerical simulation of large random matrices [16] (dots). The width $\sigma(x)$ of the Gaussian distribution of level shifts together with the x^2 asymptotics at small x is shown in the inset.

$$c(x)=\int_{-\infty}^{\infty}d\omega\int_0^{2\pi}\frac{d\phi}{2\pi}\frac{1}{z_+z_-}(-\partial_x^2)Z(\omega,x;\phi), \qquad (3)$$

$$p(\omega,x)=\int_0^{2\pi}\frac{d\phi}{2\pi}\frac{1}{z_+z_-}(-\partial_\omega^2)Z(\omega,x;\phi), \qquad (4)$$

where $z_\pm(\phi)=1+e^{\pm i\phi}$ and, adopting the shorthand notation $\mathbb{1}$ to represent the Dirac δ function,

$$Z(\omega,x;\phi)=\det_{[-1,1]}[\mathbb{1}-\hat{\mathcal{K}}(\phi)]. \qquad (5)$$

The operator kernel $\hat{\mathcal{K}}(\phi)$ has matrix elements

$$\mathcal{K}(\lambda,\mu;\phi)=\frac{1}{4\pi i}\sqrt{\mathcal{D}(\lambda)\mathcal{D}(\mu)}\,\frac{F(\lambda;\phi)-F(\mu;\phi)}{\lambda-\mu}, \qquad (6a)$$

where

$$F(\lambda;\phi)=\frac{(z_++z_-)}{\pi i}⨍_{-\infty}^{\infty}d\mu\frac{\mathcal{D}^{-1}(\mu)}{\mu-\lambda}-(z_+-z_-)\mathcal{D}^{-1}(\lambda). \qquad (6b)$$

Here the integral is understood in the sense of the Cauchy principal value, with variables λ and μ restricted to the interval $[-1,1]$, and the dependence on x and ω is encoded in the function

$$\mathcal{D}(\lambda)=\exp[i\pi\omega\lambda+\pi^2x^2\lambda^2/2]. \qquad (7)$$

It is interesting to note that, after the substitution $x^2\mapsto -it$, at $\phi=0$, the integral kernel $\hat{\mathcal{K}}$ coincides with that arising in the calculation of time-dependent correlation functions of the one-dimensional interacting Bose gas at zero temperature [15]. A comparison of the universal function $c(x)$ as inferred from Eqs. (3) and (5)–(7) with the results of direct numerical simulation is shown in Fig. 1.

Before outlining the derivation of these results, several remarks are in order.

(i) The universality of Eqs. (6) can be inferred from the universality of Eq. (13) below [6]. As such, these results can be applied to the parametric evolution of spectra that obey Dyson statistics only locally.

(ii) Although we have not succeeded in obtaining a direct proof, in accordance with the conjecture made in Ref. [17], the distribution of single-level shifts appears to assume a Gaussian form $p(\omega,x)=e^{-\omega^2/2\sigma(x)}/\sqrt{2\pi\sigma(x)}$ *at any value* of x. The corresponding width of the Gaussian can be expressed as

$$\sigma(x)\equiv\langle[\epsilon_i(\overline{x}+x)-\epsilon_i(\overline{x})]^2\rangle=2\int_0^x dx'(x-x')c(x').$$

At small x, where $p(\omega,x)$ can be inferred from the level velocity distribution [6,12], $\sigma(x)\overset{x\to 0}{\sim}x^2$, which reflects (identifying time with x^2) independent "diffusion" of individual levels. In the opposite limit $x\mapsto\infty$, making use of the known asymptotic dependence [6] $c(x)\overset{x\to\infty}{\sim}-1/\pi^2x^2$ obtained from a perturbative analysis, one can infer the limiting behavior $\sigma(x)\overset{x\to\infty}{\sim}\text{const}+(2/\pi^2)\ln x$. The resulting strongly subdiffusive behavior at large x can be ascribed to the rigidity of the spectrum "hemming in" the meandering levels.

(iii) The generating function Z is a particular case of a more general object $\tilde{Z}_q(J,J';x;\phi)$ which defines

$$P_q(J,J';x)=\int_0^{2\pi}\frac{d\phi}{2\pi}e^{iq\phi}\tilde{Z}_q(J,J';x;\phi) \qquad (8)$$

as the probability that the number $n(J)$ of levels $\{\epsilon_i(\overline{x})\}$ in the (not necessarily contiguous) interval J and the number $n'(J')$ of levels $\{\epsilon_i(\overline{x}+x)\}$ in the interval J' differ by exactly q. Taking J and J' to be semi-infinite intervals $J_\epsilon=(-\infty,\epsilon]$ and $J_{\epsilon+\omega}=(-\infty,\epsilon+\omega]$, one can derive generalizations of Eqs. (3) and (4), which involve correlations between levels $\epsilon_i(\overline{x})$ and $\epsilon_{i+q}(\overline{x}+x)$:

$$\begin{aligned}c_q(x)&\equiv\langle\partial_{\overline{x}}\epsilon_i(\overline{x})\partial_{\overline{x}}\epsilon_{i+q}(\overline{x}+x)\rangle\\&=(-1)^q\int_{-\infty}^{\infty}d\omega\int_0^{2\pi}\frac{d\phi}{2\pi}\frac{e^{iq\phi}}{z_+z_-}(-\partial_x^2)\\&\quad\times\tilde{Z}_q(J_\epsilon,J_{\epsilon+\omega};x;\phi),\end{aligned} \qquad (9)$$

$$\begin{aligned}p_q(\omega,x)&\equiv\langle\delta[\epsilon_{i+q}(\overline{x}+x)-\epsilon_i(\overline{x})-\omega]\rangle\\&=(-1)^q\int_0^{2\pi}\frac{d\phi}{2\pi}\frac{e^{iq\phi}}{z_+z_-}(-\partial_\omega^2)\tilde{Z}_q(J_\epsilon,J_{\epsilon+\omega};x;\phi).\end{aligned} \qquad (10)$$

The exact analytic expression for $\tilde{Z}$ will be given below.

(iv) In some applications, the fixed perturbation XV may be of *finite rank*; that is, it may possess only a finite number r of nonzero eigenvalues [18]. In such situations Eqs. (6)

retain their validity providing $\mathcal{D}(\lambda)$ is replaced by $e^{i\pi\omega\lambda}\,\mathrm{det_{sc}}(1-i\lambda\mathcal{R})$, where $\mathcal{R}$ is the reactance matrix for scattering of the potential XV [13], and $\mathrm{det_{sc}}$ denotes the determinant in the space of scattering channels. In this case, x may be identified with any of the variables parametrizing $\mathcal{R}$.

(v) Despite the existence of well-developed analytical tools for the study of integral kernels with the *structure* of Eq. (6a) [15], it is at present unclear whether these methods can be generalized to accommodate ϕ integration in Eqs. (3) and (4).

The analysis of parametric statistics of individual energy levels relies on a technical device which ensures that the level $\epsilon_i(\overline{x}+x)$ is indeed the descendant of $\epsilon_i(\overline{x})$ by demanding that it has the same ordinal number as counted from the bottom of the spectrum. Specifically, due to the absence of level crossings, the intralevel velocity correlation function coincides with the conditional average

$$c(x)=\int_{-\infty}^{\infty}d\omega\Big\langle\,\delta_{n(J_\epsilon),n'(J_{\epsilon+\omega})}\sum_{ij}\,\partial_{\overline{x}}\theta[\epsilon-\epsilon_i(\overline{x})]\times\partial_{\overline{x}}\theta[\epsilon+\omega-\epsilon_j(\overline{x}+x)]\Big\rangle, \tag{11}$$

where $\delta_{n,n'}$ denotes the Kronecker δ symbol, and θ is the step function. The corresponding distribution of level shifts $p(\omega,x)$ is given by an analogous expression with $\partial_{\overline{x}}$ replaced by ∂_ϵ (and no integration over ω). By generalizing the corresponding nonparametric formula for $P_n(J)$ [19], our starting point is the general expression for the probability $P_{nn'}(J,J')$ to find n levels in the interval J of the unperturbed sequence *and* n' levels in the interval J' of the perturbed sequence,

$$P_{nn'}(J,J')=\frac{(-1)^{n+n'}}{n!n'!}\sum_{k=n}^{\infty}\sum_{k'=n'}^{\infty}\frac{(-1)^{k+k'}r_{kk'}}{(k-n)!(k'-n')!}. \tag{12}$$

Here $r_{kk'}$ represents the multipoint parametric correlation function of the DOS [6,18] integrated over the interval $J^k\otimes J'^{k'}$ with the corresponding measures $d\mu_J$ and $d\mu_{J'}$. Owing to the determinantal structure of the DOS correlation function, $r_{kk'}$ can be represented in the form of a fermionic functional integral

$$r_{kk'}=\det K\int\mathcal{D}\Psi\,\mathcal{D}\overline{\Psi}\left(\int d\mu_J(u)\overline{\xi}(u)\xi(u)\right)^k\times\left(\int d\mu_{J'}(w)\overline{\eta}(w)\eta(w)\right)^{k'}\times\exp\left[\int du\int dw\overline{\Psi}(u)K^{-1}(u,w)\Psi(w)\right], \tag{13}$$

where $\overline{\Psi}=(\overline{\xi},\overline{\eta})$ is a fermionic doublet. Here

$$\hat{K}=\begin{pmatrix}\hat{k} & \hat{\mathcal{D}}_0^{-1}[\hat{k}-\mathbb{1}]\\ \hat{\mathcal{D}}_0\hat{k} & \hat{k}\end{pmatrix}, \tag{14}$$

where the matrix elements of the operator sine kernel $\hat{k}$ of the unitary Dyson ensemble are $k(u-w)=\sin\pi(u-w)/\pi(u-w)$, and $[\hat{\mathcal{D}}_0\hat{k}](u,w)=e^{-(x^2/2)d^2/du^2}k(u-w)$. Fixing the difference $n'-n=q$ and summing over all n, one obtains the probability $P_q(J,J';x)$ that the numbers of levels in the two intervals J and J' differ by q:

$$P_q(J,J';x)=\sum_{n=0}^{\infty}\frac{1}{n!(n+q)!}\sum_{\substack{k=n\\k'=n+q}}^{\infty}\frac{(-1)^{k+k'+q}r_{kk'}}{(k-n)!(k'-n-q)!}=\int_0^{2\pi}\frac{d\phi}{2\pi}e^{iq\phi}\sum_{\substack{k=0\\k'=q}}^{\infty}\frac{(-1)^{k+k'+q}r_{kk'}}{k!k'!}z_+^kz_-^{k'}. \tag{15}$$

Substituting Eq. (13) into Eq. (15), one finds

$$P_q(J,J';x)=(-1)^q\int_0^{2\pi}\frac{d\phi}{2\pi}e^{iq\phi}\Bigg\{\det[\mathbb{1}\sigma_0-\hat{K}\Pi(\phi)]-\sum_{k'=0}^{q-1}\frac{\partial_\gamma^{k'}}{k'!}\det[\mathbb{1}\sigma_0-\hat{K}\Pi_\gamma(\phi)]\Bigg|_{\gamma=0}\Bigg\}, \tag{16}$$

where

$$\Pi(\phi)=\begin{pmatrix}z_+ & 0\\ 0 & z_-\end{pmatrix},\quad \Pi_\gamma(\phi)=\begin{pmatrix}z_+ & 0\\ 0 & \gamma z_-\end{pmatrix},$$

and σ_i are the Pauli matrices. The determinants are understood as functional determinants on the space of two-component functions defined on the product interval $J\otimes J'$. The expression in curly brackets in Eq. (16) can be identified as the generating function $\tilde{Z}$.

In order to apply Eq. (16) to the computation of the intralevel velocity correlation function and the distribution of the parametric level shifts, one must set $J=J_\epsilon$ and $J'=J_{\epsilon+\omega}$. Setting $q=0$ and using Eq. (11), one obtains Eqs. (3) and (4), where Z is identified with the first determinant in Eq. (16). For $q\neq 0$, a similar procedure leads to Eqs. (9) and (10).

The use of semi-infinite intervals to define $n(J_\epsilon)$ and $n'(J_{\epsilon+\omega})$ is justified only if the support of the spectrum is finite. The latter condition would be trivially fulfilled if one were to use, instead of $k(u-w)$, the exact Christoffel-Darboux kernel whose scaling limits interpolate between the sine kernel inside the Wigner semicircle, and the Airy kernel at its endpoints. However, in practice, employing such a kernel would present significant technical difficulties. To circumvent this problem, we use a regularized kernel

$$k_\delta(u-w)=\frac{\sin\pi(u-w)}{\pi(u-w)}e^{-(1/2)\delta(|u|+|w|)}, \tag{17}$$

where the limit $\delta\to 0$ is implied in all expressions involving this kernel. Using Eq. (13) it is easily shown that $\langle n(J_\infty)\rangle=\langle n'(J_\infty)\rangle=2/\delta$, and $\langle[n(J_\infty)-n'(J_\infty)]^2\rangle\sim O(\delta)$. Thus, although the regularization formally violates the level number conservation, the corresponding error tends to zero in the limit $\delta\to 0$. In the following we will suppress the index δ.

As written, Eq. (16) involves a matrix oscillating integral kernel defined on a product of semi-infinite intervals. However, as we will now show for the case $q=0$, it can be rewritten in the form of Eqs. (6) which is (i) more amenable to numerical analysis, and (ii) makes the integrability of the kernel (in the sense discussed in Ref. [15]) manifest. Without loss of generality, we can set $\epsilon=0$, and shift the variables so as to define the determinant on the quadrant $(-\infty,0]\otimes(-\infty,0]$. The corresponding shift operator is absorbed into the redefinition $\hat{\mathcal{D}}_0\to\hat{\mathcal{D}}=e^{\omega d/du}\hat{\mathcal{D}}_0$. The term involving the δ function in the upper right corner of Eq. (14) can be separated to reveal the dyadic structure of the remainder:

$$\hat{K}=\begin{pmatrix}\mathbb{1}\\ \hat{\mathcal{D}}\end{pmatrix}\otimes(\hat{k}\quad \hat{\mathcal{D}}^{-1}\hat{k})-\begin{pmatrix}0 & \hat{\mathcal{D}}^{-1}\mathbb{1}\\ 0 & 0\end{pmatrix}.$$

Now, using the identities $(\mathbb{1}\sigma_0+z_-\hat{\mathcal{D}}^{-1}\mathbb{1}\sigma_+)^{-1}=(\mathbb{1}\sigma_0-z_-\hat{\mathcal{D}}^{-1}\mathbb{1}\sigma_+)$, and $\det(\mathbb{1}\sigma_0+z_-\hat{\mathcal{D}}^{-1}\mathbb{1}\sigma_+)=1$, where $\sigma_+=(\sigma_1+i\sigma_2)/2$, one obtains

$$\det[\mathbb{1}\sigma_0-\hat{K}\Pi(\phi)]=\det\{\mathbb{1}-[z_+\hat{k}-z_+z_-\hat{k}(\hat{\mathcal{D}}^{-1}\mathbb{1})\hat{\mathcal{D}}+z_-(\hat{\mathcal{D}}^{-1}\hat{k})\hat{\mathcal{D}}]\}.$$

Employing the Fourier representations,

$$\begin{Bmatrix}k(u)\\ \delta(u)\end{Bmatrix}=\frac{1}{2}\int_{-\infty}^{\infty}d\lambda\begin{Bmatrix}\theta(1-\lambda)\theta(1+\lambda)\\ 1\end{Bmatrix}e^{i\lambda\pi u}$$

and making use of Eq. (7), one finds

$$[z_+\hat{k}-z_+z_-\hat{k}(\hat{\mathcal{D}}^{-1}\mathbb{1})\hat{\mathcal{D}}+z_-(\hat{\mathcal{D}}^{-1}\hat{k})\hat{\mathcal{D}}](u,w)=\int_{-1}^{1}\frac{d\lambda}{2}e^{i\pi\lambda(w-u)}\Bigg\{z_+-\frac{z_+z_-}{2\pi i}\int_{-\infty}^{\infty}d\mu\times\frac{e^{i\pi w(\mu-\lambda)}\mathcal{D}^{-1}(\mu)}{\lambda-\mu-i\delta}\hat{\mathcal{D}}+z_-\mathcal{D}^{-1}(\lambda)\hat{\mathcal{D}}\Bigg\}. \tag{18}$$

Finally, the cyclic invariance of the determinant and the identity $z_++z_-=z_+z_-$ are used to perform the integrals in the u-w space, with the resulting kernel in the λ-μ space having the form of Eqs. (6). Remarkably, taking the limit $\delta\to 0$ in the final expressions leads to a *nonsingular* kernel defined in terms of the Cauchy principal value integral (6b).

As a final comment, it should be noted that the method of using the ϕ integration to "count" the levels in conjunction with the regularization analogous to Eq. (17) is equally applicable to other Dyson ensembles. However, at present there exist no analogs of Eq. (13) for other ensembles, and thus our consideration is perforce limited to the unitary case.

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[19] Equation (12) is a straightforward generalization of the nonparametric object $P_n(J)$ (see, e.g., Appendix 7 of Ref. [2]).